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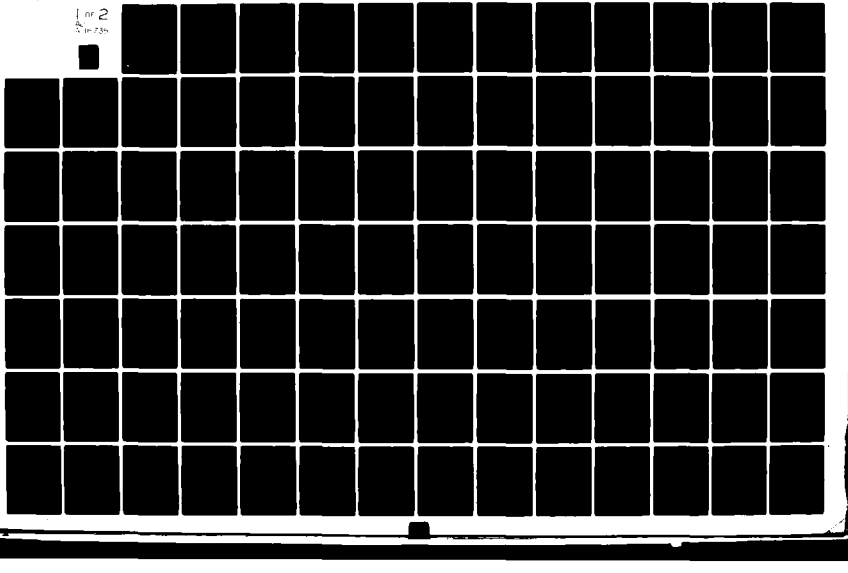

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Abstract

PRECONDITIONING STRATEGIES FOR SOLVING ELLIPTIC
DIFFERENCE EQUATIONS ON A MULTIPROCESSOR

Charles Kirkland Taft, Jr.
Captain, United States Air Force
Master of Science
Department of Computer Science
University of Illinois
157 pages

This thesis deals with choosing preconditioning strategies to accelerate a conjugate gradient algorithm for solving elliptic difference equations, suitable for implementation on a multiprocessor. The hypothetical multiprocessor considered consists of p linearly connected processors. A variety of popular preconditioning strategies for sequential machines are examined. Numerical experiments are conducted and recommendations made.

PRECONDITIONING STRATEGIES FOR SOLVING ELLIPTIC DIFFERENCE EQUATIONS ON A MULTIPROCESSOR

BY

CHARLES KIRKLAND TAFT, JR.

B. S., University of New Hampshire, 1976

THESIS

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THIS IS TO CERTIFY THAT THE CONTENT, FORMAT, AND QUALITY OF PRESENTATION OF THE THESIS SUBMITTED BY CHARLES KIRKLAND TAFT, JR. AS ONE OF THE REQUIREMENTS FOR THE DEGREE OF MASTER OF SCIENCE IS ACCEPTABLE TO THE DEPARTMENT OF COMPUTER SCIENCE
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Appendices

1. Introduction

My thesis deals with solving systems of linear equations

$$Ax = b, \tag{1.1}$$

where A is a sparse symmetric and positive definite matrix. Systems of this type arise from the discretization of second order self-adjoint elliptic partial differential equations. Many direct and iterative numerical methods have been developed for solving this problem; see for example [Varg62], [Wach66], [Youn71], [HaYo81] and [Birk81]. The advent of multiprocessor systems brings with it the possibility of substantial speedup in performing these types of numerical methods. This would allow us to examine problems that, until now, had been too large or complex to be computationally feasible. The new multiprocessor systems will require that new numerical methods be generated or that older methods be modified to take full advantage of their potential.

In this paper I consider only the conjugate gradient method and preconditioning strategies that are best suited for implementation on a multiprocessor system. The hypothetical multiprocessor that will be considered consists of p linearly connected processors as shown in figure 1.1.

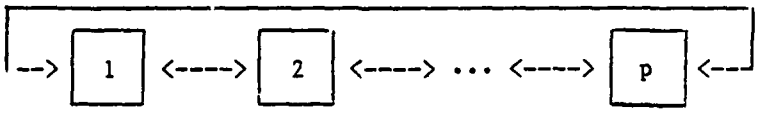


Figure 1.1

Each processor is assumed to be capable of performing any arithmetic operation in one time step, and that it takes ψ time steps to transfer one floating point number from one processor to either of its neighbors.

For sequential machines, the problem of preconditioning the conjugate gradient algorithm has been extensively studied in the liturature. See for example [AxGu80], [CoGO76], [Eise81], [Gust78], [HaYo81], [Kers78], [Mant80], [MeVo77], [Munk80], [Reid71], and [Reid72].

2. Model Problem

Consider the second order self-adjoint partial differential equations of the form

$$-\frac{\partial}{\partial x}\left[a(x,y)\frac{\partial u}{\partial x}\right] - \frac{\partial}{\partial y}\left[c(x,y)\frac{\partial u}{\partial y}\right] + f(x,y)u = g(x,y) \qquad (2.1)$$

with $a(x,y) > 0$, $c(x,y) > 0$ and $f(x,y) \geq 0$; defined on the unit square, $0 \leq x,y \leq 1$; and with boundary conditions of the form

$$\alpha u + \beta\frac{\partial u}{\partial n} = \gamma \qquad (2.2)$$

where $\frac{\partial u}{\partial n}$ is the derivative normal to the boundary.

Superimposing a square grid of mesh size $h = 1/(n+1)$ and using central difference approximations to the derivatives, the problem converts to solving a linear system of equations of order n^2. This process is fully derived and explained in [Varg62]. Handling boundary conditions of the form (2.2) where $\beta \neq 0$ is discussed in [MiGr80].

Under certain boundary conditions, the resulting coefficient matrix A is a positive definite M-matrix [Vors81]. An M-matrix is defined such that given matrix $A = (a_{ij})$,

1) $a_{ii} > 0$ 2) $a_{i,j} \leq 0$

3) A^{-1} exists 4) $A^{-1} \geq 0$.

In Appendix D, I will describe the nature of matrix A for each of my test problems. The structure of matrix A is determined by the grid point ordering scheme. Appendix A shows examples of the natural, point red/black, line red/black and 2 line red/black ordering schemes and the resulting structure of the matrix A for n=6.

3. Background

3.1. Conjugate Gradient Method

The Conjugate Gradient (CG) Method was developed by Hestenes and Stiefel in 1952. The idea behind it is to approximate the solution vector x by

$$x^{(m)} = x^{(0)} + \sum_{j=1}^{m} \alpha_j v_j$$

where

$x^{(0)}$ is an arbitrary initial guess, the vectors v_j are A-conjugate (ie. $v_j^T A v_i = 0$ for $j \neq i$) and the α_j's are chosen to minimize $||x^{(m)} - x||_A$ where $||z||_A = (z, Az)^{1/2}$.

The vectors v_{j+1} are constructed by orthogonalizing the residual $r_j = b - Ax^{(j)}$ with respect to v_j, ie. $r_j^T v_i = 0$ for $j > i$. In this way, each iteration is attempting to minimize the components of the residual r_i along the eigenvector corresponding to the most extreme eigenvalue. The residual then lies almost entirely in the subspace of the eigenvectors with the remaining less extreme eigenvalues. The iteration proceeds as if the most extreme eigenvectors and eigenvalues were not present [Kers78].

In the absence of round-off errors, the CG method can be considered a direct method, in that it will converge to the true solution of a system of order n in exactly n steps, due to the orthogonality of the

vectors v_j. In fact, if the n×n matrix A has only r distinct eigenvalues, then the method converges in only r steps. Many times, the relative error $||x^{(i)} - x||/||x||$ will be quite small even for $i \ll n$. Unfortunately, in the presence of round-off errors, the orthogonality of the vectors v_i can break down and the guaranteed finite convergence is lost. It was this breakdown that prevented the CG method from getting much attention. It wasn't until 1971 that interest was renewed in the CG method. At that time, Reid [Reid71] showed that the CG algorithm is very effective for handling large and sparse positive definite linear systems as arise from our model problem. Its cause was further helped when Concus, Golub and O'Leary [CoGO76] showed that it could be used as an effective tool for accelerating the convergence of various iterative methods. They pointed out that the CG method possesses some very attractive properties:

1) doesn't require prior knowledge of extreme eigenvalues to calculate optimal convergence parameters

2) takes advantage of the entire distribution of eigenvalues of matrix A

3) is optimal in the class of all algorithms for which $x^{(k+1)} = x^{(0)} + P_k(K)r^{(0)}$ where $K = I - M^{-1}N$, $A = M - N$ is a regular splitting and $P_k(\xi)$ is a polynomial of degree k, in the sense that it minimizes $||x_{k+1} - x||_A$.
See [CoGO76] for more details.

The rate of convergence of the CG algorithm depends heavily on the distribution of eigenvalues of matrix A. The fewer distinct eigenvalues or the more clustered the eigenvalues, the quicker the convergence. Unfortunately, the matrices arising from our model problem tend to have eigenvalue distributions that are widely distributed with little clustering. As a result, the CG algorithm by itself tends to do poorly. This situation can be improved by "preconditioning" matrix A.

3.2. Preconditioning

The idea behind preconditioning is to obtain a matrix C such that C is positive definite and $C^{-1}A$ has a "better" eigenvalue distribution. It is also important to choose matrix C such that solving a system $Cw = q$ is as easy as possible. The CG algorithm is then applied to the new preconditioned system

$$C^{-1}Ax = C^{-1}b.$$

This notation has one problem in that $C^{-1}A$ may no longer be symmetric. It is better to consider the preconditioned system

$$(C^{-1/2}AC^{-1/2})(C^{1/2}x) = C^{-1/2}b, \text{ or}$$

$$(L^{-1}AL^{-T})(L^{T}x) = L^{-1}b,$$

$$\text{where } C = LL^{T}.$$

Obviously the best eigenvalue distribution for $C^{-1}A$ would be achieved when $C = A$, then $C^{-1}A = I$. This does not help us much, however, in that solving a system $Cw = q$ is no easier than solving the

original system. The idea then is to choose matrix C as close as possible to A, such that $C^{-1}A$ would have a few extreme eigenvalues with the rest clustered around unity, while still requiring $Cw = q$ be easy to solve.

When matrix A is an M-matrix, Meijerink and van der Vorst [MeVo77] introduced a set of preconditioning strategies based on an incomplete factorization of matrix A. The idea is to choose $C = LU$, such that matrix C resembles matrix A, $A = C - R$, with L and U almost as sparse as matrix A. The sparsity of L and U is controlled by forcing certain predetermined positions within L and U to be zero. These positions are defined by a set P of places (i,j) such that

$$P \subset P_n \equiv \{ (i,j) \mid i \neq j \; 1 \leq i \leq n, \; 1 \leq j \leq n \}$$

where P_n contains all pairs of indices of

off-diagonal matrix elements.

When matrix A is symmetric, we add the restriction to the set P that if $(i,j) \in P$ then so must $(j,i) \in P$ and consider an incomplete Cholesky factorization (LL^T or LDL^T). Meijerink and van der Vorst proved that if matrix A is an M-matrix, then this process is stable and the resulting factorization

$$C = LL^T \text{ or } LDL^T$$

is positive definite.

Using this set P notation, we can describe most of the basic preconditioning strategies. On the extremes, we have $P = P_n$ and $P = \phi$

which result in diagonal scaling, $C = diag(A)$ and preconditioning by complete Cholesky factorization, $C = A$, respectively. In between we have

$$P^* \equiv \{ (i,j) \mid A(i,j)=0 \}$$

which is the preconditioning strategy used by the ICCG(0) algorithm of Meijerink and van der Vorst [MeVo77].

When Matrix A is positive definite, but not an M-matrix, non-positive or small diagonal elements can result during the factorization process, causing matrix C to be no longer positive definite. A number of modifications have been proposed to solve this problem. Kershaw [Kers78] recommends simply replacing the non-positive diagonal elements by suitable positive numbers. He has found that a few diagonal elements can become non-positive and be so replaced without distracting from the incomplete factorization, as long as most of the pivots remain positive. Another approach is simply to add αD to matrix A before attempting the incomplete factorization, where $D = diag(A)$ and α is a positive scalar. This idea was proposed by Manteuffel [Mant80] in developing his shifted incomplete Cholesky factorization. If α is large enough, then the factorization is guaranteed to be positive definite. However, choosing α too large results in very slow convergence of the resulting conjugate gradient algorithm. Unfortunately, the only way to determine a "good" value of α for a given problem is through trial and error. For the test problems considered by Manteuffel, good results were achieved for α of $O(10^{-2})$.

A number of variations on the incomplete factorization idea of Meijerink and van der Vorst have been proposed. Gustafsson [Gust78] introduced the concept of the modified incomplete factorization. Here the elements created during the incomplete factorization that correspond to entries in the set P are added to the diagonal elements of matrix C prior to being discarded. The process is known as diagonal modification. The MICCG(0) algorithm results when adding diagonal modification to the ICCG(0) algorithm. Gustafsson reports that a faster asymptotic rate of convergence can be achieved.

Another variation has been proposed by Munksgaard [Munk80]. Here, instead of dropping a predetermined set of elements P during the factorization, he proposes developing criteria for dropping only the "smaller" fill-ins while retaining the "larger" ones. The philosophy here is that the number of iterations required to reach a solution is more sensitive to the size of the elements dropped than to the number dropped. He suggests dropping fill-in elements if their numeric value relative to the diagonal elements of their row and column is less than a relative drop tolerance. In the k^{th} pivot step we drop $l_{i,j}^{(k+1)}$ if

$$|l_{ij}^{(k+1)}| < c(d_{ii}^{(k)} d_{jj}^{(k)})^{1/2}.$$

The amount of fill-in is determined by the size of c. If c is close to zero, we obtain almost a complete factorization, while c = 1 produces a factorization where no fill-ins are added and L has the same sparsity pattern as matrix A.

3.3. Preconditioned Conjugate Gradient Method

Given a preconditioning matrix C and an initial guess x_0, the standard preconditioned conjugate gradient (PCG) method can be described in the following algorithmic format:

Algorithm 3.1

a) Initial step

1) $r_0 = b - Ax_0$

2) $z_0 = C^{-1}r_0$

3) $p_0 = z_0$

b) For k = 0, 1, ...

1) $\alpha_k = (r_k, z_k)/(p_k, Ap_k)$

2) $x_{k+1} = x_k + \alpha_k p_k$

3) $r_{k+1} = r_k - \alpha_k Ap_k$

4) $z_{k+1} = C^{-1}r_{k+1}$

5) $\beta_k = (r_{k+1}, z_{k+1})/(r_k, z_k)$

6) $p_{k+1} = z_{k+1} + \beta_k p_k$.

A commonly used stopping criterion for this algorithm is to calculate $||r_k|| = (r_k, r_k)^{1/2}$ each iteration and stop when $||r_k|| < \varepsilon$, where ε

is a user specified parameter.

One choice for the initial iterate x_0 is a random vector. A more creative approach is to choose $x_0 = C^{-1}b$. This uses the fact that if matrix C is close to matrix A, then $x_0 = C^{-1}b$ will be a reasonably accurate estimate for $x = A^{-1}b$. Starting with a more accurate estimate for x will hopefully reduce the number of iterations required to generate an answer of desired accuracy.

The ICCG(0) and MICCG(0) algorithms utilize incomplete LDL^T factorization of the form

$$C = (\tilde{D} + L)\tilde{D}^{-1}(\tilde{D} + L)^T, \tag{3.1}$$

where $A \equiv L + D + L^T$, L is strictly lower triangular and D and $\tilde{D}$ are positive diagonal matrices. To define $\tilde{D}$, I will use figure A5 and use a_i, b_i and c_i to denote the elements of the main diagonal, upper-diagonal and m^{th} upper diagonal respectively, where i is the row index and m is the half band width of the matrix. Then $\tilde{D} = \text{diag}(\tilde{d}_1, \cdots, \tilde{d}_n)$ is defined for ICCG(0) as:

$$\tilde{d}_i = a_i - b_{i-1}^2 \tilde{d}_{i-1}^{-1} - c_{i-m}^2 \tilde{d}_{i-m}^{-1}$$
$$(i = 1, 2, \cdots, n)$$

and for MICCG(0) as:

$$\tilde{d}_i = a_i - b_{i-1}^2 \tilde{d}_{i-1}^{-1} - c_{i-m}^2 \tilde{d}_{i-m}^{-1} - r_i - r_{i-m+1}$$
$$r_i = c_{i-1} b_{i-1} \tilde{d}_{i-1}^{-1}$$
$$(i = 1, 2, \cdots, n)$$

where in both cases, elements not defined (ie. subscripts < 0) should be replaced by zeroes. For those algorithms where the incomplete LDL^T factorization can be described in the form (3.1), Eisenstat [Eise81] proposes a different implementation of our standard PCG Algorithm 3.1. His method reduces the number of multiply-adds required per iteration by a factor approaching one half. This is done by restating the original problem (1.1) in the form

$$[(\tilde{D} + L)^{-1}A(\tilde{D} + L)^{-T}][(\tilde{D} + L)^{T}x] = [(\tilde{D} + L)^{-1}b]$$

or

$$\hat{A}\hat{x} = \hat{b}. \tag{3.2}$$

It can then be shown that applying PCG to (1.1) with preconditioning (3.1) is equivalent to applying PCG to (3.2) with preconditioning $C = \tilde{D}^{-1}$ and setting $x = (\tilde{D} + L)^{-T}\hat{x}$. The algorithm can now be written as:

Algorithm 3.2

a) Initial step

1) $\hat{r}_0 = (\tilde{D} + L)^{-1}(\hat{b} - \hat{A}x_0)$

2) $\hat{p}_0 = \hat{z}_0 = \tilde{D}\hat{r}_0$

b) For k = 0, 1, ...

1) $\hat{\alpha}_k = (\hat{r}_k, \hat{z}_k)/(\hat{p}_k, \hat{A}\hat{p}_k)$

2) $x_{k+1} = x_k + \hat{\alpha}_k(\tilde{D} + L)^{-T}\hat{p}_k$

3) $\hat{r}_{k+1} = \hat{r}_k - \hat{\alpha}_k\hat{A}\hat{p}_k$

4) $\hat{z}_{k+1} = \tilde{D}\hat{r}_{k+1}$

5) $\hat{\beta}_k = (\hat{r}_{k+1}, \hat{z}_{k+1})/(\hat{r}_k, \hat{z}_k)$

6) $\hat{p}_{k+1} = \hat{z}_{k+1} + \hat{\beta}_k\hat{p}_k$

To calculate $\hat{A}\hat{p}_k$, the matrix $\hat{A}$ does not have to be explicitly calculated. The product can be computed efficiently by taking advantage of the following identity:

$$\hat{A}\hat{p}_k = (\tilde{D} + L)^{-1}[(\tilde{D} + L) + (\tilde{D} + L)^T - (2\tilde{D} - D)](\tilde{D} + L)^{-T}\hat{p}_k$$

This can be simplified, and results in the following two step calculation:

$$\hat{t}_k = (\tilde{D} + L)^{-T}\hat{p}_k$$

$$\hat{A}\hat{p}_k = \hat{t}_k + (\tilde{D} + L)^{-1}(\hat{p}_k - K\hat{t}_k),$$

where $K \equiv 2\tilde{D} - D$.

This version requires 8N + NZ(A) multiply-adds, versus 6N + 2NZ(A) for Algorithm 3.1, where NZ(A) = number of non-zero elements in matrix A. Another 3N multiply-adds can be saved by symmetrically scaling the problem so that $\tilde{D} = I$, [Eise81].

Rutishauser considered a version of the PCG algorithm, where x_i and r_i are calculated using a 3-term recurrence relation. It can be represented in the following algorithmic format:

Algorithm 3.3

a) Initial step

1) choose initial guess x_0

2) $x_{-1} = 0$

3) $\omega_1 = 1$

4) $r_0 = b - Ax_0$

5) $z_0 = C^{-1}r_0$

b) For $k = 0, 1, \cdots$

1) $\alpha_k = (z_k, r_k)/(z_k, Cz_k)$

2)

$$\omega_{k+1} = 1/[1 - \frac{\alpha_k}{\alpha_{k-1}} \frac{(z_k, r_k)}{(z_{k-1}, r_{k-1})} \omega_k^{-1}] \quad (k>1)$$

3) $x_{k+1} = x_{k-1} + \omega_{k+1}(\alpha_k z_k + x_k - x_{k-1})$

4) $r_{k+1} = r_{k-1} + \omega_{k+1}(-\alpha_k Az_k + r_k - r_{k-1})$

5) $z_{k+1} = C^{-1} r_{k+1}$.

This version is particularly useful when considering the conjugate gradient method as a means of accelerating other iterative methods, as in [CoGO76]. In general, Reid [Reid71] showed that this version required more storage to implement than does our standard PCG algorithm 3.1.

When matrix A possesses "Property A", Reid [Reid72] showed how algorithm 3.3 could be modified to reduce the amount of work per iteration by approximately one half. In general, the same results can be obtained if our problem (1.1) can be partitioned such that:

$$\begin{bmatrix} C_1 & F \\ F^T & C_2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}. \tag{3.3}$$

This can also be represented by the two matrix equations:

$$C_1 x_1 = b_1 - F x_2 \tag{3.4}$$

$$C_2 x_2 = b_2 - F^T x_1. \tag{3.5}$$

The idea behind Reid's modification is to choose an initial guess $x_1^{(0)}$ and then use it to calculate $x_2^{(0)}$ via (3.5). This then implies that $z_2^{(0)}$ and forces $\alpha_0 = 1$, where I assume z is partitioned in the same fashion as (3.3). A simple inductive argument shows that for $j = 0, 1, 2, \cdots$

$$\alpha_j = 1 \text{ and } z_1^{(2j+1)} = z_2^{(2j)} = 0.$$

As a result, algorithm 3.3 can be reduced to:

Algorithm 3.4

a) Initial step

1) choose initial guess $x_1^{(0)}$

2) $\omega_1 = 1$

3) $x_2^{(0)} = C_2^{-1}(b_2 - F^T x_1^{(0)})$

4) $r_1^{(0)} = (b_1 - Fx_2^{(0)}) - C_1 x_1^{(0)}$

5) $z_1^{(0)} = C_1^{-1} r_1^{(0)}$

6) $\theta_1^{(0)} = (z_1^{(0)}, r_1^{(0)})$

b) For k = 0, 1, 2, ...

1)

$$r_2^{(2k+1)} = (1 - \omega_{2k+1}) r_2^{(2k-1)} - \omega_{2k+1} F^T z_1^{(2k)}$$

2) $z_2^{(2k+1)} = C_2^{-1} r_2^{(2k+1)}$

3) $\theta_2^{(2k+1)} = (z_2^{(2k+1)}, r_2^{(2k+1)})$

4)

$$\omega_{2k+2} = [1 - \omega_{2k+1}^{-1} \theta_2^{(2k+1)} / \theta_1^{(2k)}]^{-1}$$

5)

$$\Delta x_1^{(2k)} = \omega_{2k+1}\omega_{2k+2}[z_1^{(2k)} + (1 - \omega_{2k}^{-1})(1 - \omega_{2k+1}^{-1})\Delta x_1^{(2k-2)}]$$

6) $x_1^{(2k+2)} = x_1^{(2k)} + \Delta x_1^{(2k)}$

7)

$$r_1^{(2k+2)} = (1 - \omega_{2k+2})r_1^{(2k)} - \omega_{2k+2}Fz_2^{(2k+1)}$$

8) $z_1^{(2k+2)} = C_1^{-1}r_1^{(2k+2)}$

9) $\theta_1^{(2k+2)} = (z_1^{(2k+2)}, r_1^{(2k+2)})$

10)

$$\omega_{2k+3} = [1 - \omega_{2k+2}^{-1}(\theta_1^{(2k+2)}/\theta_2^{(2k+1)})]^{-1}$$

c) Once $x_1^{(m)}$ has been obtained to the desired accuracy, calculate $x_2^{(m)}$ using:

$$x_2^{(m)} = C_2^{-1}(b_2 - F^T x_1^{(m)}).$$

The main advantages with this approach are that the algorithm is working with 1/2 the number of unknowns each iteration, and that each iteration of Algorithm 3.4 is equivalent to two iterations of Algorithm 3.3.

4. Investigative Process

4.1. Introduction

The investigation will be divided into three phases. In the first phase I examine a group of preconditioning strategies arising from the ideas of Meijerink and van der Vorst, Gustafsson, and Munksgaard, and determine how they compare to one another on a given set of problems. The preconditioning strategies will be judged on how they influence the eigenvalue distribution of our test matrices, and their effect on the rate of convergence and amount of work required by a standard CG algorithm to obtain a given relative error.

The second phase consists of analyzing each preconditioning strategy and determining which ones might be easily adaptable to our multiprocessor system. A prime consideration is to identify those preconditioning strategies that minimize the total amount of work, including the amount of interprocessor communication required to construct the preconditioning matrix C and to solve the systems $z = C^{-1}r$.

From the results of the first two phases, I will narrow the list of possible strategies to two or three prime candidates for preconditioning on multiprocessors. The third phase then consists of analyzing the effects of these strategies on larger and more complex test problems. I will also examine what effect various values of ψ, the interprocessor

communications cost parameter, might have on our choice of a preconditioning strategy. The numerical experiments required during Phase I and Phase III will be conducted on the CDC-Cyber 175 at the University of Illinois, for which the arithmetic precision is roughly 14 decimal digits.

4.2. Software

In conducting the numerical experiments, I relied heavily on the Harwell sparse matrix routines MA31 and EA14A. The MA31 package served as the basis for the incomplete factorization and conjugate gradient routines. A complete description of these routines can be found in [Munk80]. The program listings and on-line write-ups for the MA31 package are available in the Cyber Harwell library under the name MA31A.

The conjugate gradient routine MA31F, contained in this package, was slightly modified. Originally, it chose as its initial guess

$$x_0 = C^{-1}b.$$

In order to make it more difficult for the algorithm and to get a better idea of how the preconditioning would effect convergence, I replaced b by a vector *with random entries between 0 and 2.*

The eigenvalues of our symmetrically preconditioned matrices were found using a Lanczos algorithm as implemented in the Harwell routine EA14A. This algorithm finds the eigenvalues without regard to their multiplicity. A complete description of this routine can be found in

[PaRe81]. The only modification made was to replace the Harwell random number function FA01AS by the CDC Fortran function RANF. The complete program listings and write-ups for this routine should be available shortly in the Cyber Harwell library.

This routine requires that the user supply the necessary code to calculate $u = u + Av$ each iteration, where the subroutine EA14A supplies the vectors u and v. Since we are working with a symmetrically preconditioned matrix A, we actually need to calculate

$$u = u + L^{-T}AL^{-1}v \tag{4.1}$$

where $C = LL^T$.

This was done using the Harwell subroutines Ma31G and MA31H. The subroutine MA31G solves the system

$$x = (LL^T)^{-1}y$$

using backward and forward substitution. I broke this into two separate subroutines; MA31G1 to do the backward substitution, and MA31G2 to do the forward substitution. The subroutine MA31H is used to calculate $Ax = y$. Using these three routines, we can solve equation (4.1) in the following four steps:

1) solve $t_1 = L^{-1}v$ using MA31G2

2) calculate $t_2 = At_1$ using MA31H

3) solve $t_3 = L^{-T} t_2$ using MA31G1

4) calculate $u = u + t_3$.

Appendix F contains source listings for the programs I created, and those Harwell routines which I modified.

4.3. Preconditioning Strategies

The following is a list of abbreviations and descriptions of the preconditioning strategies that I have examined.

1) DS - Diagonal Scaling

This method uses C = diag(A) as its preconditioning matrix.

2) BDS - Block Diagonal Scaling

Similar to diagonal scaling, this method uses C = block diag(A), where each principle submatrix is tri-diagonal.

3) IC(s) - Incomplete Cholesky factorization with s diagonals added

This technique was developed by Meijerink and van der Vorst [MeVo77]. It is normally associated with matrices generated using the natural grid point ordering scheme. The case when no fill-ins are kept during the factorization (s=0), can easily be generalized for matrices using other grid point ordering schemes. Here I will limit myself to the cases s = 0, 1 and 3. They utilize set P's of

the form:

$$P^0 \equiv \{(i,j) \mid A(i,j) = 0 \}$$

$$P^1 \equiv \{(i,j) \mid |i-j| \neq 0,1,m-1,m \}$$

$$P^3 \equiv \{(i,j) \mid |i-j| \neq 0,1,2,m-2,m-1,m \}$$

where m is the half band width of the outer diagonal.

4) MIC(s) - Modified Incomplete Cholesky factorization with s diagonals added

Developed by Gustafsson [Gust78], it represents an extension of the IC(s) algorithm to include diagonal modification.

5) HARWELL(c) - Harwell package MA31 with drop tolerance c

This performs the incomplete Cholesky factorization as proposed by Munksgaard [Munk80] and implemented by the Harwell routine MA31C. It uses a numeric drop tolerance to control fill-ins, and includes diagonal modification. It also incorporates minimum degree pivoting to minimize the number of potential fill-ins generated. I will limit myself to the two cases c=0 and $c=10^{-2}$. The case c=0 generates a complete Cholesky factorization.

6) MICD(c) - Modified Incomplete Cholesky factorization with Drop tolerance c

Similar to the HARWELL(c) algorithm, in this case the minimum degree pivoting has been eliminated.

7) RBIC(s) - Reduced Block Incomplete Cholesky factorization with s diagonals added

This is similar to the IC(s) algorithm, except that only portions of matrix A are used to calculate the incomplete Cholesky factorization. Parts of matrix A are ignored in order to break matrix A into n/2 uncoupled systems of equations. The incomplete Cholesky factorization on each system can then be performed independently. Using the notation in Appendix B, the following is how the matrices arising from the various grid point ordering schemes will be partitioned:

a) Point Red/Black Ordering (Figure B4)

The elements in blocks E_i, E_i^T, F_i and F_i^T $(i = 1,\ldots,(\frac{n}{2} - 1)$ will be ignored during the factorization.

b) Line Red/Black Ordering (Figure B2)

The elements in blocks E_{2i} $(i = 1,\ldots,(\frac{n}{2} - 1))$ will be ignored.

c) 2 Line Red/Black Ordering (Figure B3)

The elements in blocks E_{2i} $(i = 1,\ldots,(\frac{n}{2} - 1))$ will be ignored.

I will limit myself to the case s=0, except when working with the 2 Line Red/Black matrices, where I will also examine the case s=3.

Each of these preconditioning strategies was not necessarily matched with each of the grid point ordering schemes. Table 4.1 shows which combinations were examined.

Preconditioning Strategy	Grid Point Ordering Schemes			
	Natural	Point R/B	Line R/B	2-line R/B
DS	X	X		
BDS	X		X	X
IC(0)	X	X	X	X
IC(1)	X			
IC(3)	X			
MIC(0)	X	X	X	X
MICD(10^{-2})	X	X	X	X
MICD(0)	X	X	X	X
HARWELL(10^{-2})	X	X	X	X
HARWELL(0)	X	X	X	X
RBIC(0)		X	X	X
RBIC(3)				X

Table 4.1

4.4. Phase I

4.4.1. Introduction

During this phase, I was interested in determining how the various chosen preconditioning strategies compare to one another. I limited myself to comparing them relative to test matrices of order 64 arising from test problem 1 with n=8 (see appendix D). Appendix C outlines which combinations of preconditioning strategies and grid point ordering schemes I looked at.

A prime consideration when choosing an algorithm for this type of problem is the amount of work required to generate an acceptable answer. Keeping this in mind, I determined the amount of time and number of iterations required by our PCG algorithm to produce an answer such that

$$||r_i|| < 10^{-6}$$

$$\text{where } r_i = Ax_i - b.$$

This was subdivided into the time required to compute the preconditioning matrix and that required to actually perform the PCG iterations.

Another means of comparing preconditioning strategies is to examine their effect on the eigenvalue distribution of the test matrices. Ideally, the eigenvalues of the symmetrically preconditioned test matrices should be clustered around one. In an effort to gauge this, I used the Harwell routine EA14A to calculate all the distinct eigenvalues

(λ_i) of the symmetrically preconditioned matrices to an accuracy of 10^{-4}. I then calculated the range, mean and standard deviation of (λ_i - 1.0). The more successful the strategy, the closer these values will be to zero.

The conclusions reached during this phase are not necessarily intended to hold for larger and more complex problems. A much wider variety and size of test problems would have to have been considered. Such a comprehensive study is beyond the scope of this paper. More exhaustive studies comparing various subsets of these preconditioning strategies with respect to sequential machines only can be found in [MeVo77], [Gust78], and [Munk80].

4.4.2. Software

A modified version of the Harwell incomplete factorization routine MA31C will be used to generate all the various types of factorizations required during this phase. As written, it performed the incomplete factorization using a numeric drop tolerance, diagonal modification, and minimum degree pivoting. To allow the routine to handle a wider variety of factorizations, I made the minimum degree pivoting and diagonal modification user controlled options. I also allowed the user to choose either a numeric drop tolerance or a user defined function FILL to control fill-ins. The function FILL would decide if a zero should be

destroyed by considering only its coordinates, and would be similar in nature to the set P of Meijerink and van der Vorst [MeVo77].

The routine MA31A, used to activate MA31C, was also changed. It had been used to prepare the data structures required during the incomplete factorization. Its duties were taken over by my routine FACTOR. Eliminated was the automatic diagonal scaling of matrix A. This necessitated a change to another Harwell routine MA31H, used to calculate $Ax = y$. No longer does this routine assume $Diag(A) = I$. I also added to FACTOR an option to allow the user to specify which portions of matrix A would be used in calculating the incomplete factorization. This was done using a user defined function EUSE which, when activated, identifies which portion of matrix A is to be passed on to subroutine MA31C.

It should be noted that, while these modifications do allow a greater variety of preconditioning strategies to be implemented, the process at times is far from efficient. As a result, the time required to perform some of the incomplete factorizations will be inflated. This is especially true for the IC(s) and RBIC(s) factorizations. Normally, the locations of the non-zero entries in the factorization are known beforehand, and only those values need be calculated. Here, most of the work required to generate a potential fill-in is done before the program decides to keep it or not. This results in more values being calculated than need be.

The execution time of the factorization (MA31C) and the preconditioned conjugate gradient (MA31F) routines will be determined using the CDC Fortran function SECOND. This function returns the central processor time from start-of-job in seconds. The difference between the values recorded at the start and end of a routine will be its execution time. The values returned by function SECOND are usually accurate to two decimal places.

The statistics on the calculated eigenvalues will be generated using the CDC Math/Science Library routines DSCRPT and DSCRP2. The source code for both routines is in the Cyber MSL Library.

4.4.3. Results

The results of the numerical experiments have been tabulated and placed in Tables 4.2 - 4.9 and Graphs 4.1 - 4.5 at the end of this section. First, I will discuss some general observations about the data. I will then look at each preconditioning strategy separately, discuss how it relates to the other preconditioning strategies, and what effect the different grid point ordering schemes may have had upon it.

There exists a definite correlation between the number of iterations required to solve the preconditioned system and the size of the spectral radius, and the range and standard deviation of the resulting eigenvalues. The smaller the spectral radius, the range, and

the standard deviation of the eigenvalues, the fewer the number of iterations. In most cases, the mean is also reasonably close to zero. This supports the idea that the closer the eigenvalues of the symmetrically preconditioned matrix are clustered around one, the faster the method will converge. Such observations, however, did not hold for the MIC(0) preconditioning strategy. Unfortunately, I have not been able to explain why. From this data, it is clear that the distribution, rather than the number of distinct eigenvalues is the characteristic relevant to the rate of convergence. In fact, the non-preconditioned matrix is the matrix with the fewest distinct eigenvalues.

As a result of the relatively small size of our test system, the times consumed by the various preconditioned C.G. algorithms are clustered together. If any method could be classified as the fastest, the Harwell(10^{-2}) would probably be the one. It registered a time of 0.03 second when matched with the point red/black matrix and the 2-line red/black matrix. From this data alone however, it is difficult to conclude whether the difference in times resulting from the various ordering schemes is significant. When the Harwell(10^{-2}) method is compared to its sister method MICD(10^{-2}), the benefits of minimum degree pivoting (Harwell(10^{-2})) are clearly evident. In each case, the Harwell(10^{-2}) method produced better results in every category than did the MICD(10^{-2}) method. The MICD(10^{-2}) method also proved extremely sensitive to the type of ordering scheme used.

Had the IC(n) methods been more efficiently implemented, they would have matched the efficiency of the Harwell(10^{-2}) method. That aside, they were still very competitive. The IC(0) method proved to be a substantial improvement over the BDS method in all areas. The results for the IC(0) method fluctuate slightly depending on the grid point ordering scheme used. It is unclear whether or not these changes are significant. Additional tests would have to be conducted. The IC(1) method made modest additional improvements to both the eigenvalue distribution and rate of convergence. The timing data between the IC(0) and IC(1) methods is so close, that it is impossible to tell which is more efficient. The IC(3) method, on the other hand, while making additional improvements on the eigenvalue distribution, did not improve the rate of convergence enough to outweigh the increased cost of the factorization. As a result, it is less desirable than the IC(0) or IC(1) methods. However, the results of Meijerink and van der Vorst [MeVo77] show that for larger systems, the IC(3) method is indeed superior. How the IC(3) method would compare to the Harwell(10^{-2}) method on larger systems has, to my knowledge, not been thoroughly explored.

The MIC(0) method proved extremely sensitive to the type of grid point ordering scheme used. It had the most trouble with the point red/black matrix. Here the process became unstable and six diagonal elements had to be changed, using Kershaw's technique [Kers78], to keep the factorization positive definite. On the other hand, with a

naturally ordered matrix, it seemed to be fairly competitive as far as the time required to obtain an answer. The eigenvalue distribution, however, suffered as compared to the IC(n) methods. While the data here indicates the MIC(0) method slightly inferior to the IC(0) method, Gustafsson [Gust78], using naturally ordered matrices, showed that for larger systems the MIC(n) methods required fewer iterations than the corresponding IC(n) methods.

The Harwell(0) method seems to be surprisingly competitive, considering that it represents a complete factorization. However, the results of Munksgaard [Munk80] show that, as would be expected, this competitiveness *does not extend to larger systems*. When compared to the other complete factorization method, MICD(0), the benefits of minimum degree pivoting are again clearly evident. In each case, the Harwell(0) method produced fewer fill-ins and required substantially less time to perform the factorization. Another interesting observation is that the Harwell(0) method was not influenced by the grid point ordering scheme used, while the MICD(0) was definitely sensitive to the ordering scheme used. For the MICD(0) method, the number of elements in the lower triangular part of the factorization varied from 584 to 326. This was reflected in the time required to calculate the factorization, which varied accordingly.

The DS and BDS methods were somewhat disappointing. The DS method, while improving the eigenvalue distribution tremendously, did little to

improve the rate of convergence associated with our conjugate gradient routine. The BDS method was equally ineffectual. It produced almost no improvement in the eigenvalue distribution over the DS method, and only a modest improvement in the rate of convergence. Unfortunately, this improvement in the rate of convergence was overshadowed by the cost of the factorization. As we will see in section 4.6.3, the BDS method is not as worthless as these results would indicate.

The RBIC(0) method proved to be reasonably successful. Where they could be compared, its results fall almost exactly half way between those of the BDS and IC(0) methods. Only minor fluctuations in results occurred between the various grid point ordering schemes. The RBIC(3) method, on the other hand, proved to be a major disappointment. In every category, it was inferior to the RBIC(0) method. It is unclear whether these results are characteristic of the RBIC(3) method, or simply a consequence of the size of the test problem.

Natural Ordering

Preconditioning Method	FACTOR Number of Elements in L	FACTOR Time	SOLVE Number of Iterations	SOLVE Time	Total Time
None	0	0.0	24	0.05	0.05
DS	0	0.0	24	0.05	0.05
BDS	56	0.01*	20	0.05	0.06
IC(0)	112	0.01*	10	0.03	0.04
IC(1)	161	0.02*	7	0.02	0.04
IC(3)	245	0.03*	6	0.02	0.05
MIC(0)	112	0.01	11	0.03	0.04
MICD(10^{-2})	249	0.03	6	0.02	0.05
MICD(0)	455	0.07	1	0.01	0.08
HARWELL(10^{-2})	210	0.03	4	0.01	0.04
HARWELL(0)	290	0.03	1	0.01	0.04

Table 4.2 - Timing and convergence data resulting from solving the test problem.

Preconditioning Method	Spectral Radius	Number of Distinct Eigenvalues	GETEIG Statistics on (λ_i - 1.0) Range	Mean	Std. Dev.
None	8.876	33	7.518	3.00	2.059
DS	2.219	33	1.879	-0.26E-6	0.515
BDS	2.377	64	1.773	-0.32E-6	0.399
IC(0)	1.329	54	0.858	-0.0219	0.164
IC(1)	1.205	55	0.512	-0.0065	0.074
IC(3)	1.108	45	0.245	-0.0029	0.036
MIC(0)	2.960	49	1.499	0.361	0.347
MICD(10^{-2})	1.220	57	0.169	0.025	0.033
MICD(0)	1.00	1	0.0	0.0	0.0
HARWELL(10^{-2})	1.076	38	0.057	0.013	0.014
HARWELL(0)	1.00	1	0.0	0.0	0.0

Table 4.3 - Data on the eigenvalue distribution of the symmetrically preconditioned test matrix.

Point Red/Black Ordering

Preconditioning Method	FACTOR Number of Elements in L	FACTOR Time	SOLVE Number of Iterations	SOLVE Time	Total Time
DS	0	0.0	24	0.05	0.05
RBIC(0)	88	0.01*	17	0.04	0.05
IC(0)	112	0.01*	13	0.03	0.04
MIC(0)	112	0.01*	24	0.06	0.07
MICD(10^{-2})	241	0.03	5	0.02	0.05
MICD(0)	326	0.04	1	0.01	0.05
HARWELL(10^{-2})	211	0.02	4	0.01	0.03
HARWELL(0)	290	0.03	1	0.01	0.04

Table 4.4 - Timing and convergence data resulting from solving the test problem.

Preconditioning Method	Spectral Radius	Number of Distinct Eigenvalues	GETEIG Statistics on (λ_i - 1.0) Range	Mean	Std. Dev.
DS	2.194	33	1.879	0.16E-6	0.515
RBIC(0)	1.660	52	1.333	-0.004	0.346
IC(0)	1.438	31	1.172	0.033	0.292
MIC(0)	18.827	32	13.951	3.821	4.539
MICD(10^{-2})	1.129	31	0.098	0.019	0.021
MICD(0)	1.00	1	0.0	0.0	0.0
HARWELL(10^{-2})	1.076	34	0.063	0.015	0.016
HARWELL(0)	1.00	1	0.0	0.0	0.0

Table 4.5 - Data on the eigenvalue distribution of the symmetrically preconditioned test matrix.

Line Red/Black Ordering

Preconditioning Method	FACTOR Number of Elements in L	FACTOR Time	SOLVE Number of Iterations	SOLVE Time	Total Time
BDS	56	0.01*	20	0.05	0.06
RBIC(0)	88	0.01*	16	0.04	0.05
IC(0)	112	0.01*	11	0.03	0.04
MIC(0)	112	0.01	14	0.04	0.05
MICD(10^{-2})	301	0.04	6	0.02	0.06
MICD(0)	584	0.09	1	0.01	0.10
HARWELL(10^{-2})	219	0.03	4	0.01	0.04
HARWELL(0)	290	0.03	1	0.01	0.04

Table 4.6 - Timing and convergence data resulting from solving the test problem.

Preconditioning Method	Spectral Radius	Number of Distinct Eigenvalues	GETEIG Statistics on (λ_i - 1.0) Range	Mean	Std. Dev.
BDS	2.180	64	1.773	-0.150	0.399
RBIC(0)	1.722	56	1.363	-0.0047	0.321
IC(0)	1.406	61	1.000	-0.013	0.173
MIC(0)	13.192	53	9.174	0.653	1.359
MICD(10^{-2})	1.377	52	0.288	0.045	0.059
MICD(0)	1.00	1	0.0	0.0	0.0
HARWELL(10^{-2})	1.072	33	0.056	0.013	0.014
HARWELL(0)	1.00	1	0.0	0.0	0.0

Table 4.7 - Data on the eigenvalue distribution of the symmetrically preconditioned test matrix.

2-Line Red/Black Ordering

Preconditioning Method	FACTOR Number of Elements in L	FACTOR Time	SOLVE Number of Iterations	SOLVE Time	Total Time
BDS	56	0.01*	20	0.05	0.06
RBIC(0)	88	0.01*	15	0.04	0.05
RBIC(3)	164	0.02*	16	0.05	0.07
IC(0)	112	0.01*	11	0.03	0.04
MIC(0)	112	0.01	12	0.03	0.04
MICD(10^{-2})	280	0.03	7	0.03	0.06
MICD(0)	562	0.09	1	0.01	0.10
HARWELL(10^{-2})	208	0.02	4	0.01	0.03
HARWELL(0)	290	0.03	1	0.01	0.04

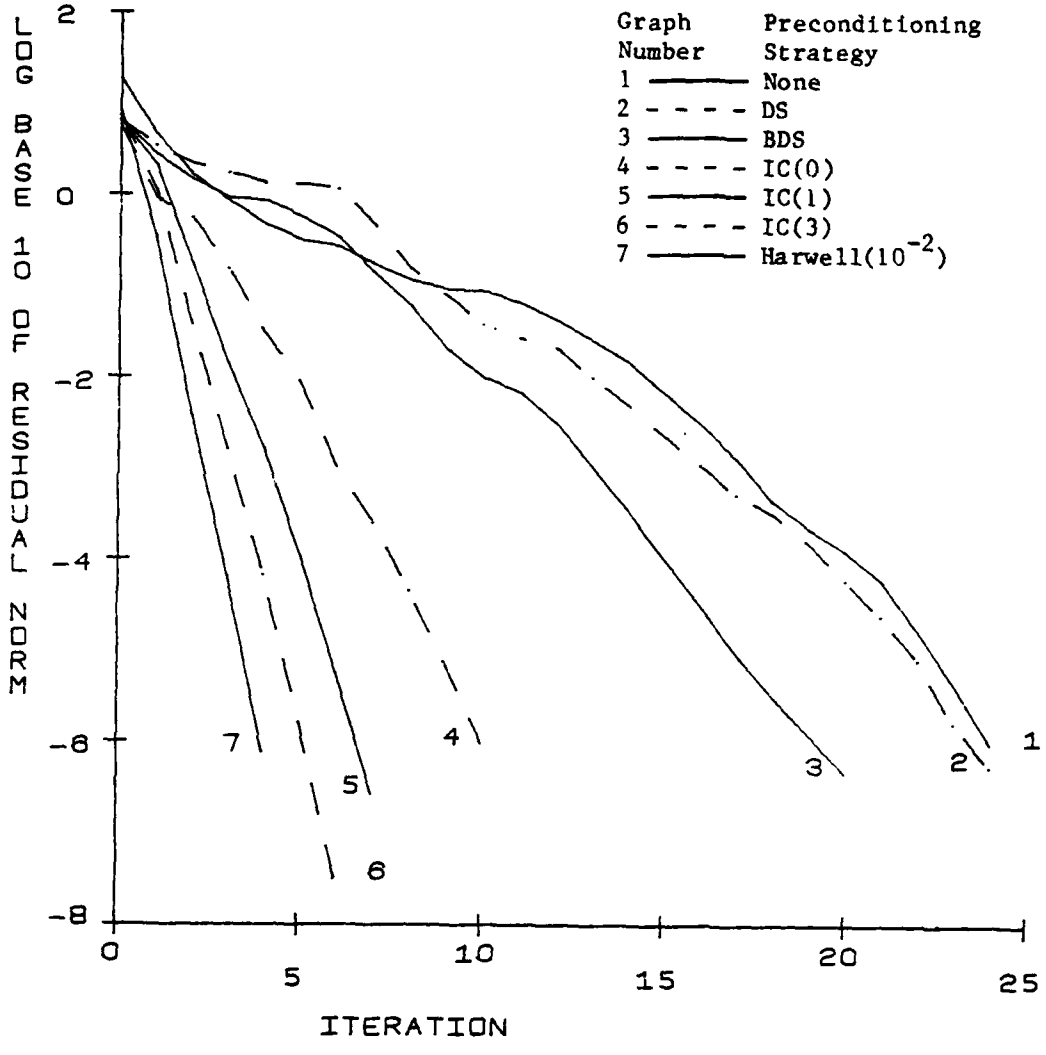
Table 4.8 - Timing and convergence data resulting from solving the test problem.

Preconditioning Method	Spectral Radius	Number of Distinct Eigenvalues	GETEIG Statistics on (λ_i - 1.0) Range	Mean	Std.Dev.
BDS	2.196	64	1.773	-0.12E-6	0.399
RBIC(0)	1.770	55	1.363	-0.004	0.324
RBIC(3)	2.052	49	1.575	-0.128E-3	0.349
IC(0)	1.319	60	0.904	^0.015	0.163
MIC(0)	5.449	51	3.341	0.440	0.562
MICD(10^{-2})	1.484	53	0.376	0.046	0.072
MICD(0)	1.00	1	0.0	0.0	0.0
HARWELL(10^{-2})	1.073	34	0.058	0.014	0.015
HARWELL(0)	1.00	1	0.0	0.0	0.0

Table 4.9 - Data on the eigenvalue distribution of the symmetrically preconditioned test matrix.

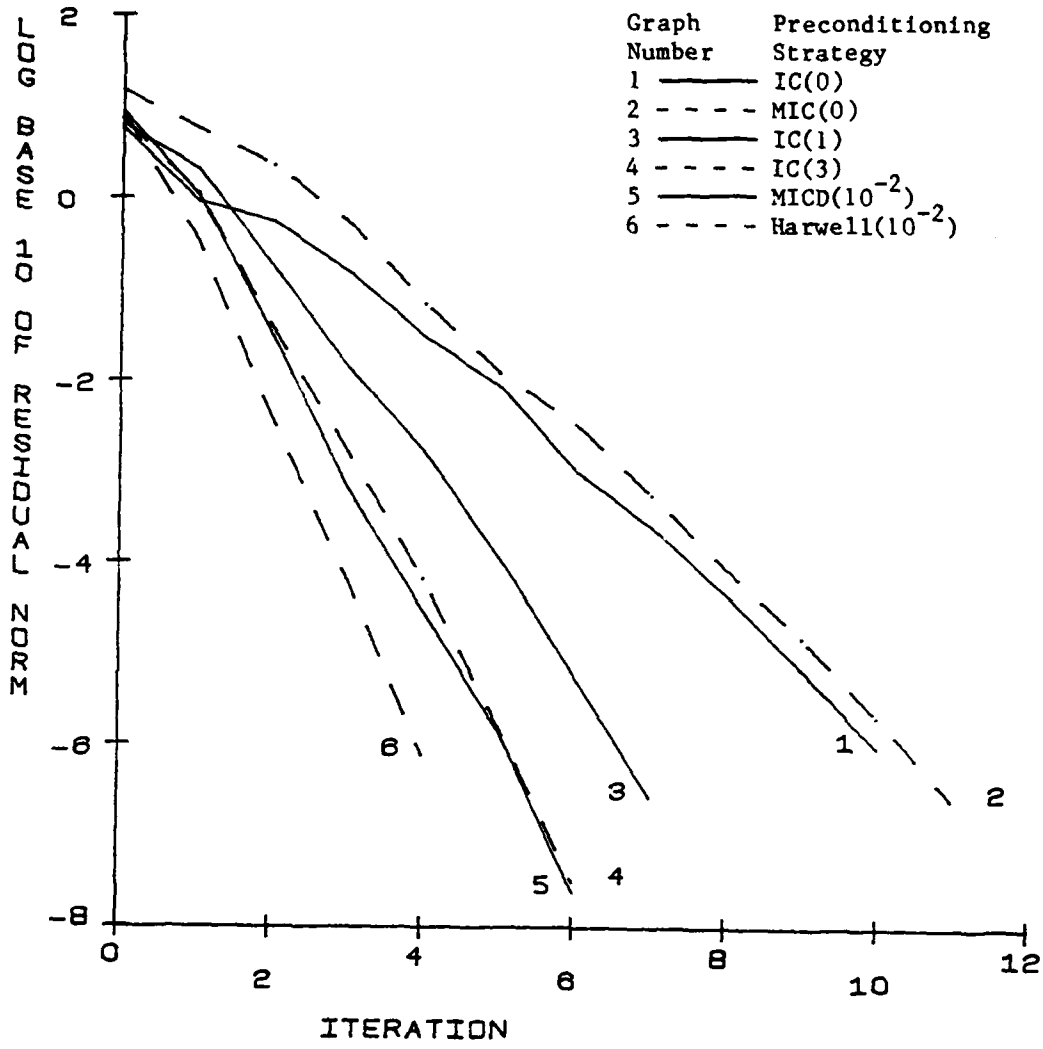
* - Tests using the routines from Phase III show that these values could be reduced by up to a factor of 3 if the corresponding preconditioning strategy had been efficiently implemented.

Natural Ordering (Part 1)



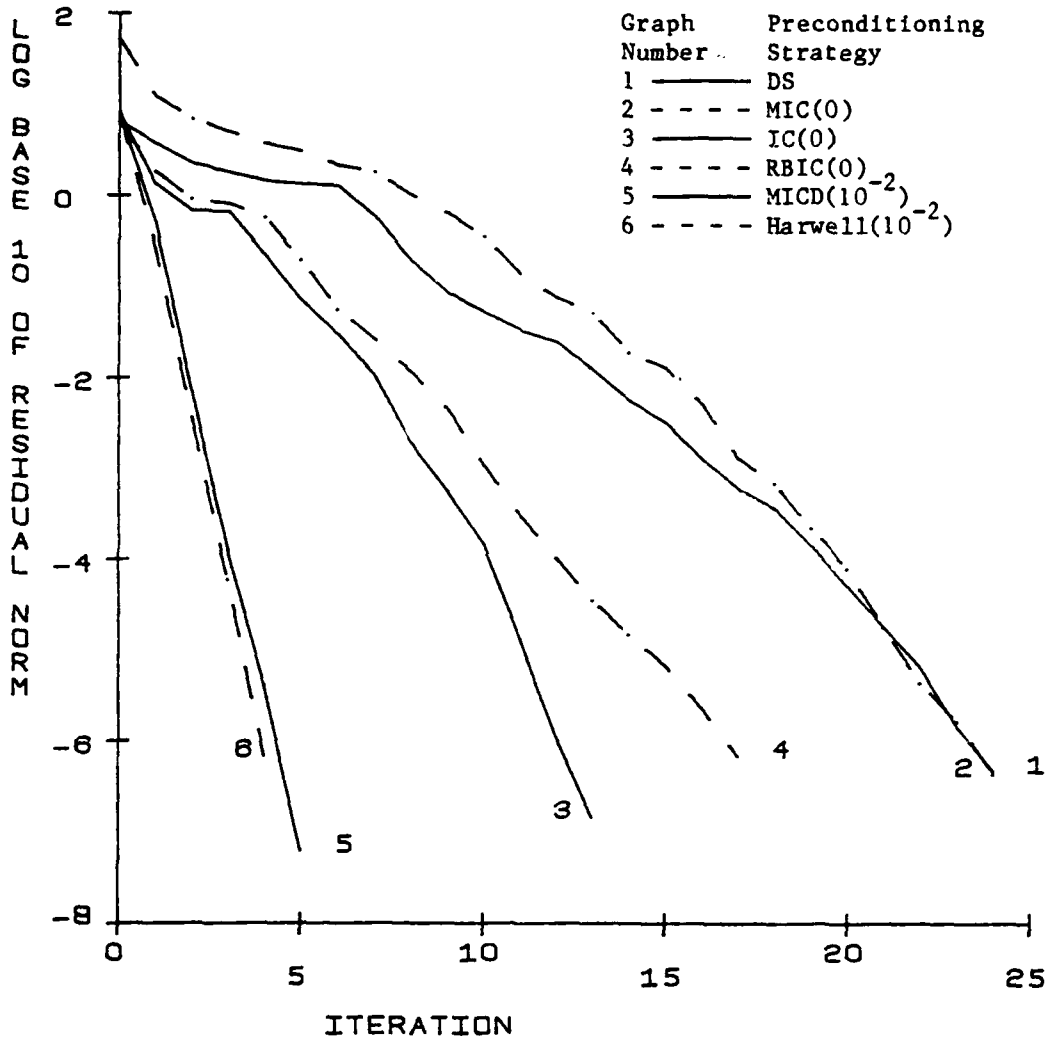
Graph 4.1 - Shows the log base 10 of the residual norm as a function of the iteration number.

Natural Ordering (Part 2)



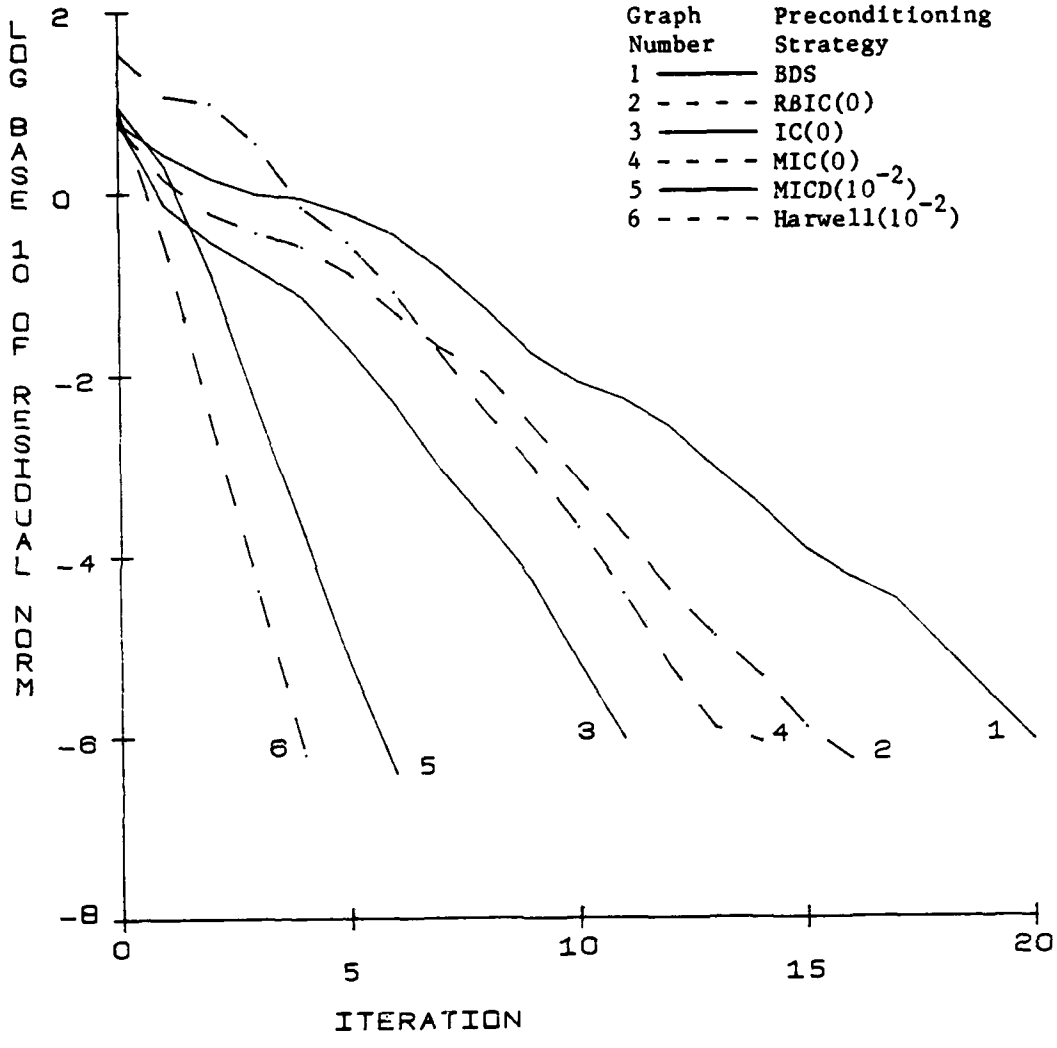
Graph 4.2 - Shows the log base 10 of the residual norm as a function of the iteration number.

Point Red/Black Ordering

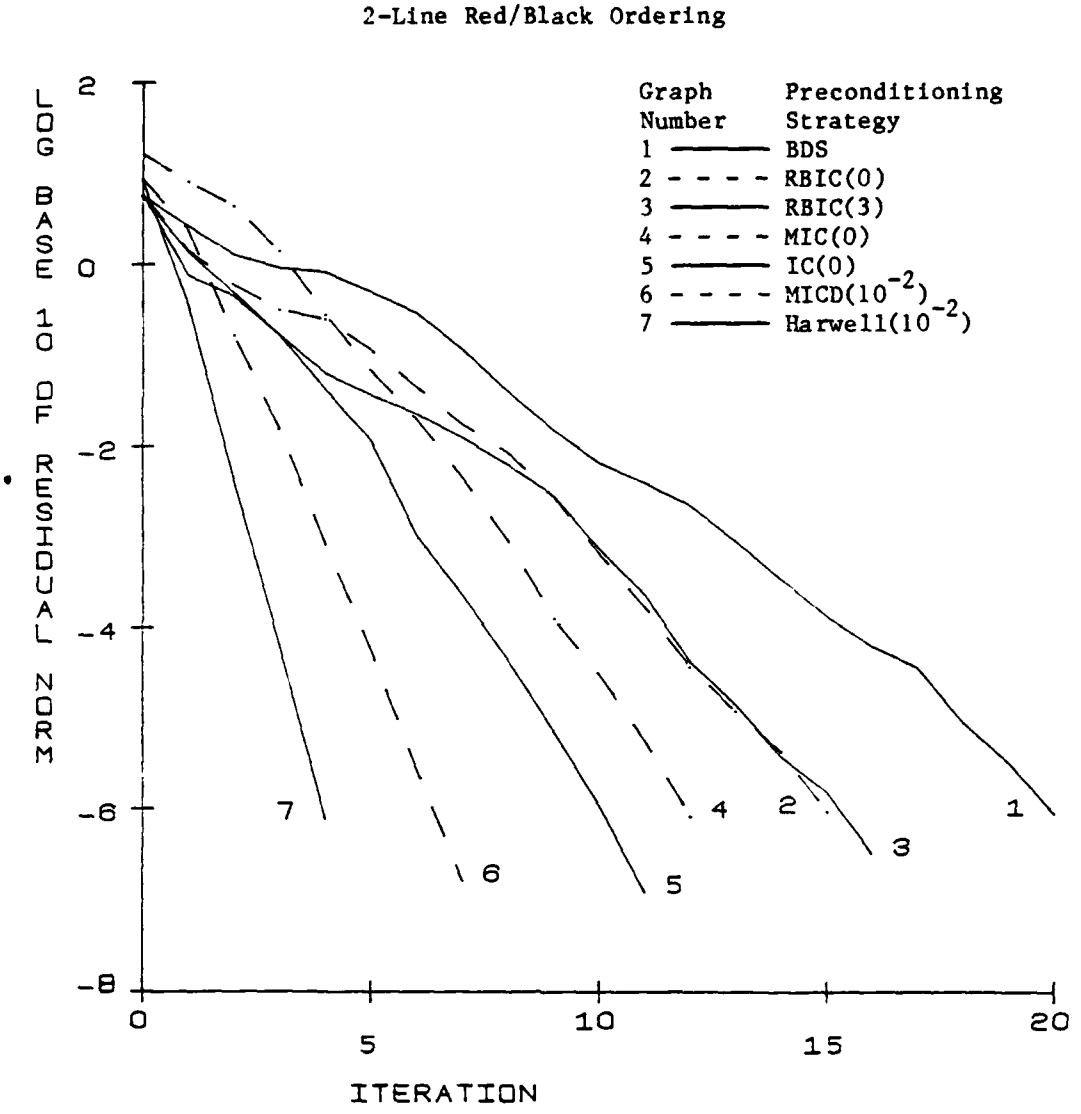


Graph 4.3 - Shows the log base 10 of the residual norm as a function of the iteration number.

Line Red/Black Ordering



Graph 4.4 - Shows the log base 10 of the residual norm as a function of the iteration number.



Graph 4.5 - Shows the log base 10 of the residual norm as a function of the iteration number.

4.5. Phase II

4.5.1. Introduction

During this phase, I attempted to analyze each of the preconditioning strategies and determine how easily they could be adapted to our multiprocessor. I assumed that matrix A is of order nm and that my multiprocessor consisted of n/2 processors (p=n/2). Under these assumptions, Table E1 (Appendix E) shows the steps involved in solving a system of equations using our preconditioned conjugate gradient algorithm. Also included are their relative cost in arithmetic operations and the amount of data that must be passed between processors. Where appropriate, the relative cost of performing a particular factorization was determined, as well as the cost of using it to solve the system of equations $z = C^{-1}r$.

As a matter of terminology, I assumed that each factorization produced a preconditioning matrix of the form

$$C = \tilde{L}\tilde{D}\tilde{L}^T$$

where $\tilde{L}$ is a unit lower triangular matrix and

$\tilde{D}$ is a positive diagonal matrix.

The system $z = C^{-1}r$ was solved using forward and backward substitution in the following manner:

$$\tilde{L}t = r$$

$$\tilde{L}^T z = \tilde{D}^{-1}t.$$

In attempting to analyze each of these events, I relied heavily on the notation defined in figures B1 - B4 of Appendix B. Furthermore, I assume that vectors x, b, r, z, and t, and matrices $\tilde{L}$ and $\tilde{D}$ are partitioned in the same manner as matrix A. Also, if matrix A contains a block E_i and an element a_{ij}, the $\tilde{E}_i$ and $\tilde{a}_{ij}$ represent the corresponding block and element in $\tilde{L}$, respectively. Figure 4.1 shows which blocks of matrix A, of the unknown vector x, and of the right-hand side vector b are stored in processor i ($i = 2,\ldots,\frac{n}{2} - 1$) for each of the grid point ordering schemes. For processor 1 and n/2, the storage requirements are slightly different, in that certain blocks mentioned in figure 4.1 are undefined. Processor i is used to calculate and store the portions of vectors r, z, and t, and matrix $\tilde{D}$ corresponding to those portions of vector x referred to in figure 4.1, as well as portions of $\tilde{L}$ that correspond to those blocks of matrix A cited in figure 4.1.

Data Initially stored in Processor i for a

Naturally Ordered Matrix	Line Red/Black Ordered Matrix	Point Red/Black Ordered Matrix	2-Line Red/Black Ordered Matrix
T_{2i-1}	T_{2i-1}	D_i	Q_i
T_{2i}	T_{2i}	$D_{i+n/2}$	F_j $j = 2\lfloor i/2 \rfloor$
E_{2i-2}	E_{2i-2}	B_i	C_k $k = 2\lceil i/2 \rceil - 1$
E_{2i-1}	E_{2i-1}	E_{i-1}	x_{2i-1}
E_{2i}	E_{2i}	E_i	x_{2i}
x_{2i-1}	x_{2i-1}	F_{i-1}	b_{2i-1}
x_{2i}	x_{2i}	F_i	b_{2i}
b_{2i-1}	b_{2i-1}	x_i	
b_{2i}	b_{2i}	$x_{i+n/2}$	
		b_i	
		$b_{i+n/2}$	

Figure 4.1

4.5.2. Results

First, I looked at those preconditioning strategies whose suitability for our multiprocessor is not influenced by the grid point ordering scheme used. These include the DS, BDS, Harwell(c) and RBIC(n) methods. The Harwell(c) method is the only one from this group that would be extremely difficult to implement. The minimum degree pivoting would require exorbitant amounts of interprocessor communications.

The remaining three methods from this group can all be easily adapted to our multiprocessor. The DS is by far the simplest. No work is required during the factorization phase, with $\tilde{L} = I$ and $\tilde{D} = \text{diag}(A)$. Solving the system $z = C^{-1}r$ is simply a matter of calculating $z_i = \tilde{D}_i^{-1} r_i$, which can be done in m arithmetic operations with no interprocessor communications required. Each processor would solve two such systems for a total of 2m arithmetic operations.

The BDS method is equally simple. Here, processor i is required to perform the factorization of two uncoupled tri-diagonal matrices (T_{2i-1} and T_{2i}). This will require ~6m arithmetic operations per processor. Solving the system $z = C^{-1}r$ is equivalent to solving n uncoupled systems of the form $z_i = T_i^{-1} r_i$ ($i = 1, \ldots, n$). Each processor will then solve two of these systems, requiring a total of ~10m arithmetic operations and no interprocessor data transfers.

The RBIC(n) method, by its very design, is ideally suited for our

multiprocessor. The n/2 uncoupled systems allow each processor to work totally independently, while performing the factorization and solving the system $z = C^{-1}r$. Each of the uncoupled systems will be of order 2m with 3m-2 non-zero off-diagonal elements in its upper triangular part. To perform the RBIC(0) factorization, each off-diagonal element a_{ij} will be involved in the following operations:

$$\tilde{a}_{ij} := a_{ij}/\tilde{d}_i$$
$$\tilde{d}_j := \tilde{d}_j - \tilde{a}_{ij}a_{ij}$$

where initially $\tilde{D}$ is set to diag(A).

This results in an expenditure of 3 arithmetic operations per off-diagonal element. Thus, the RBIC(0) factorization requires a total of ~9m arithmetic operations per processor. The RBIC(3) factorization is slightly more complicated. I assume that I am working with a 2-line red/black matrix. If $\tilde{L}^T = \text{diag}(\tilde{L}_1^T, \tilde{L}_2^T, \ldots, \tilde{L}_{n/2}^T)$, then processor i factors Q_i into $\tilde{L}_i\tilde{D}_i\tilde{L}_i^T$, where figure 4.2 shows the structure of $\tilde{L}_i^T$ and $\tilde{D}_i = \text{diag}(\tilde{d}_1, \ldots, \tilde{d}_{2m})$. The elements of $\tilde{D}_i$ and $\tilde{L}_i^T$ are calculated in the following manner:

$$\tilde{d}_j := a_j - \tilde{b}_{j-1}b_{j-1} - \tilde{g}_{j-2}g_{j-2} - \tilde{f}_{j-m+2}f_{j-m+2} - \tilde{e}_{j-m+1}e_{j-m+1} - \tilde{c}_{j-m}c_{j-m}$$

$$b_j := b_j - \tilde{e}_{j-m+1}c_{j-m+1} - \tilde{f}_{j-m+2}e_{j-m+2} - \tilde{b}_{j-1}g_{j-1} \qquad \tilde{b}_j := b_j/\tilde{d}_j$$

$$g_j := -\tilde{f}_{j-m+2}c_{j-m+2} \qquad \tilde{g}_j := g_j/\tilde{d}_j$$

$$f_j := -\tilde{b}_{j-1}e_{j-1} \qquad \tilde{f}_j := f_j/\tilde{d}_j$$

$$e_j := -\tilde{b}_{j-1}c_{j-1} \qquad \tilde{e}_j := e_j/\tilde{d}_j$$
$$\tilde{c}_j := c_j/\tilde{d}_j \qquad \tilde{a}_j := 1$$
$$\text{for } j = 1, \ldots, 2m$$

where any elements not defined (ie. subscripts < 0)

are assumed to be zero.

When simplified, we find that the RBIC(3) factorization requires ~27m arithmetic operations per processor.

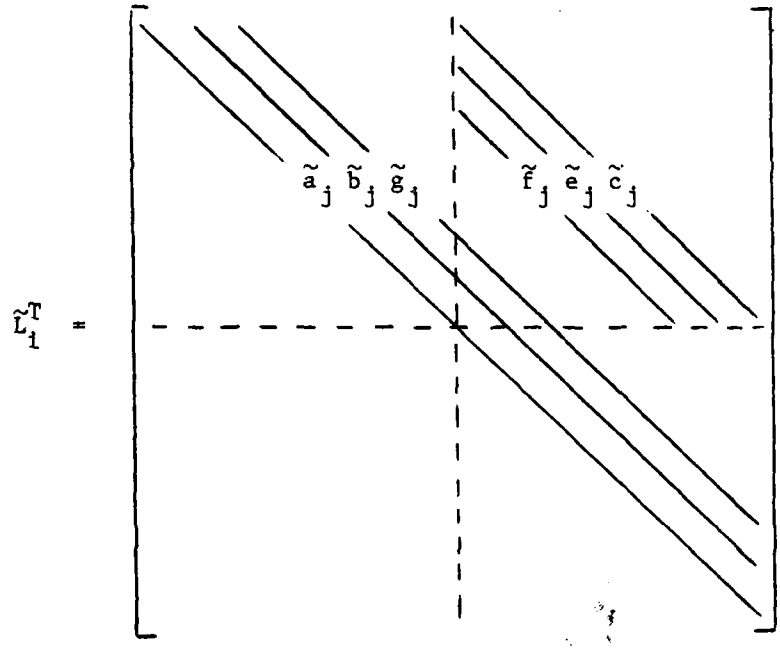


Figure 4.2

Solving $z = C^{-1}r$, when matrix C is given as $\tilde{L}\tilde{D}\tilde{L}^T$, requires approximately 2(NZL) arithmetic operations to solve $\tilde{L}t = r$ and 2(NZL) + 2m to solve $\tilde{L}^T z = \tilde{D}^{-1}t$, where NZL is the number of non-zero off-diagonal elements in $\tilde{L}$. After the RBIC(0) factorization, NZL will equal 3m-2, while after

the RBIC(3) factorization NZL will equal ~6m. This means that ~14m arithmetic operations per processor are required if the RBIC(0) is used, while if the RBIC(3) is used, ~26m arithmetic operations per processor are needed. In either case, no interprocessor data transfers are required during the factorization phase or while solving $z = C^{-1}r$.

Next, I will look at those preconditioning strategies that require a certain number of fill-ins be kept, or at least calculated, during the factorization. These methods include MICD(c), MIC(s), and IC(s) for s>0. Unfortunately, including fill-ins greatly complicates the process. They increase the interdependence between processors both during the factorization phase and while solving $z = C^{-1}r$. For example, processor i may be forced to wait for processor i-1 to finish calculating before it can proceed with its work. As a result, only a fraction of our n/2 processors may be able to operate concurrently. This greatly reduces the advantage of having those n/2 processors. The choice of grid point ordering scheme can reduce the severity of this problem somewhat, but not enough to make any of these methods suitable for our multiprocessor.

Finally we come to the IC(0) method. Unlike the other methods, its suitablity is influenced by the grid point ordering scheme used. If we are working with a naturally ordered matrix, the factorization process is recursive in nature. We find that processor i cannot start its part of the factorization process until processor i-1 has started calculating

$\tilde{D}_{2(i-1)}$. These values are needed by processor i before it can start calculating $\tilde{D}_{2i-1}$. In essence, only two processors will be able to function concurrently while performing the factorization. A similar problem arises when solving $z = C^{-1}r$.

Changing to the 2-line red/black ordering does not help the situation that much. The only advantage gained is that now $\lfloor n/4 \rfloor$ processors can be working concurrently while performing the factorization. The remaining $\lfloor n/4 \rfloor$ processors must still wait until these processors have calculated the data they need. This is still an undesirable situation.

The line red/black ordering produces a matrix much more suited for performing the IC(0) factorization on our multiprocessor. Notice that the blocks T_{2i-1} ($i = 1, \cdots, n/2$) are not directly interrelated. This means that processor i can factor T_{2i-1} without any interprocessor communication. This requires ~3m arithmetic operations. For processor i to complete the factorization, it must now get the values $\tilde{D}_{2i+1}$ from processor i+1. With these m values, processor i can finish the factorization in ~9m arithmetic operations. An additional m arithmetic operations are required to calculate $\tilde{E}_{2i-2} = \tilde{D}_{2i-1}^{-1}E_{2i-2}$. These last values will be needed by processor i to solve $z = C^{-1}r$. This makes a total of ~13m arithmetic operations and m data transfers per processor to calculate the IC(0) factorization.

Solving the system $z = C^{-1}r$ can also be easily done in this case.

During the forward substitution phase ($\tilde{L}t = r$), t_{2i-1} can be found in ~2m arithmetic operations with no interprocessor communications. The elements of t_{2i} can then be found in ~6m arithmetic operations, as long as the values t_{2i+1} are obtained from processor i+1. The backward substitution process ($\tilde{L}^T z = \tilde{D}^{-1} t$) is very similar in nature. The elements of z_{2i} are first calculated using ~3m arithmetic operations and no interprocessor communications. The values z_{2i-2} are then obtained from processor i-1. Then the values z_{2i-1} are calculated using ~7m arithmetic operations. The entire process requires a total of ~18m arithmetic operations and 2m data transfers.

The point red/black matrix is equally suited for performing the IC(0) factorization on our multiprocessor. In fact, it has one advantage over the line red/black matrix in that the factorization can be done without interprocessor communications. The structure of the point red/black matrix is such that blocks D_1 through D_k are not altered during the factorization, ie. $\tilde{D}_i = D_i$ $(i = 1, \ldots, k)$. This allows us to store those values of D_{i-1} and D_{i+1} needed by processor i during the set-up phase. Thus, if processor i has blocks B_i, E_{i-1}, E_i, F_{i-1}, F_i, D_i, $H_{(i-1)2}$, $H_{(i+1)1}$, and D_{k+i} available to it, the factorization can be performed without any data being transferred between processors. Processor i will perform the following calculations:

$$\tilde{D}_i = D_i \qquad \tilde{H}_{(i-1)2} = H_{(i-1)2} \qquad \tilde{H}_{(i+1)1} = H_{(i+1)1}$$

$$\tilde{E}_{i-1}^T = \tilde{H}_{(i-1)2}^{-1} E_{i-1}^T \qquad \tilde{F}_i^T = \tilde{H}_{(i+1)1}^{-1} F_i^T \qquad \tilde{B}_i^T = \tilde{D}_i^{-1} B_i^T$$

$$\tilde{E}_i^T = \tilde{D}_i^T E_i^T \qquad \tilde{F}_{i-1}^T = \tilde{D}_i^{-1} F_{i-1}^T$$

$$\tilde{D}_{i+k} = D_{i+k} - \text{diag}(E_{i-1}\tilde{E}_{i-1}^T) - \text{diag}(B_i\tilde{B}_i^T) - \text{diag}(F_i\tilde{F}_i^T)$$

for a total of ~13m arithmetic operations.

Solving the system $z = C^{-1}r$ will still require that some interprocessor data transfer occur. During the forward substitution phase, processor i will need from processor i-1 the m/2 elements of t_{i-1} corresponding to $H_{(i-1)2}$, and from processor i+1 the m/2 elements of t_{i+1} corresponding to $H_{(i+1)1}$. A similar set of transfers will be required during backward substitution, except involving elements from z_{i+k-1} and z_{i+k+1}. The entire process of solving $z = C^{-1}r$ will require ~18m arithmetic operations and 2m data transfers per processor.

As I have indicated, only a handful of the chosen preconditioning strategies can be efficiently implemented on our multiprocessor. The DS, BDS and RBIC(n) methods can be implemented regardless of the grid point ordering scheme used. The IC(0) method, on the other hand, is sensitive to the structure of the matrix A. Only when matrix A has a structure similar to that of the point red/black matrix or line red/black matrix can the IC(0) factorization be done efficiently. Implementation using the point red/black matrix has an added advantage in that the factorization can be performed without interprocessor communication.

4.6. Phase III

4.6.1. Introduction

From the results of Phase I and Phase II, the following combinations of preconditioning strategies and grid point ordering schemes are chosen for further analysis:

1) IC(0) with a point red/black matrix

2) BDS with a line red/black matrix

3) RBIC(0) with a 2-line red/black matrix.

For comparison purposes, I also consider a naturally ordered matrix with no preconditioning. These combinations are compared relative to test matrices of order ~1000 arising from test problem 1 (n=32), test problem 2, and test problem 3 (see appendix D). The numerical experiments are similar to those conducted during Phase I.

The size of these problems made calculating all the distinct eigenvalues of the symmetrically preconditioned test matrices extremely expensive. I therefore limit myself to examining only the extreme eigenvalues. In each case, I calculate the number of distinct eigenvalues in the interval [0.0 , 1.2]. Then, using the estimate of the spectral radius (ρ) generated by the Harwell routine EA14A, I calculate the number of distinct eigenvalues in the upper part of the spectrum defined by the interval [0.8ρ , ρ]. Of primary interest is the

number of eigenvalues that migrated into the lower part of the spectrum as a result of the preconditioning. The greater the number of eigenvalues in the interval [0.0 , 1.2], the more successful the preconditioning strategy.

Finally, the effect of different values of ϕ, the cost in time units to transfer a piece of data between neighboring processors, on the efficiency of each of the preconditioning strategies is examined. For each problem, I calculate the total number of time units required by a typical processor in our system to generate our answer. This was done using the following equation:

$$\text{Total Time} = \text{Preprocessing Time} + [\text{Number of Iterations} \times \text{Time Units per Iteration}]$$

where,

$$\text{Preprocessing Time} = \text{Number of Arithmetic Operations} + [\phi \times \text{Number of Data Transfers}],$$

$$\text{Time Units per Iteration} = \text{Number of Arithmetic Operations/iteration} + [\phi \times \text{Number of Data Transfers/iteration}].$$

Appendix E outlines the number of arithmetic operations and data transfers required by each processor to perform each step of our preconditioned conjugate gradient algorithm.

4.6.2. Software

Most of the software used during this phase is similar to that used during Phase I. However, more efficient routines BDIAG, ICCG0, and RBIC0 are developed to implement the BDS, IC(0), and RBIC(0) factorizations, respectively. Each of these three routines is based on the following algorithm:

Algorithm 4.1

1) $\tilde{D} = \text{diag}(A)$

2) For i = 1 to N do

3) For $j \in R_i^A$ do

4) $\tilde{l}_{ij} = a_{ij}/\tilde{d}_i$

5) $\tilde{d}_j = \tilde{d}_j - \tilde{l}_{ij}a_{ij}$

where N = order(A), and

set R_i^A defines which columns in row i are to be used in calculating the factorization.

For these three routines, the following is how set R_i^A is defined:

BDS - $R_i^A = \{ j \mid j=i+1 \text{ and } a_{ij} \neq 0 \}$

IC(0) - $R_i^A = \{ j \mid i<j \text{ and } a_{ij} \neq 0 \}$

RBIC(0) - $R_i^A = \{ j \mid i<j \leq i+m \text{ and } a_{ij} \neq 0 \}$.

4.6.3. Results

The data from the numerical experiments can be found at the end of this section. Tables 4.10, 12, and 14 contain the timing and convergence data pertaining to solving each of the test problems. Tables 4.11, 13, and 15 contain the corresponding data on the extreme eigenvalues of the symmetrically preconditioned test matrices. Graphs 4.6 - 4.8 show the $\log_{10}$ of the norm of the residual as a function of the iteration number. Graphs 4.9 - 4.11 show what effect the interprocessor communications cost (ϕ) can have on the amount of work required by each processor to calculate an acceptable answer.

Notice that in these cases, the time required to perform the desired factorization is trivial when compared to that required to actually solve the system. This would indicate that the savings incured by using the point red/black ordering with the IC(0) method, as opposed to using the line red/black ordering or block cyclic reduction, may not be that significant in the long run. However, unless circumstances dictate otherwise, there is no reason not to utilize the point red/black ordering and enjoy what savings it can provide.

For these test problems, the RBIC(0) method prove at least an equal to the IC(0) method in efficiency. Only in the case of test problem 1 does the IC(0) prove more efficient than the RBIC(0) method. The two methods are extremely close in the number of iterations required to solve the test problems. The RBIC(0), therefore, has a slight advantage

in that each iteration requires fewer arithmetic operations due to the fewer non-zero elements in the upper triangular part of its factorization. The BDS method is consistently a distant third, though it does represent a improvement over no preconditioning.

Unfortunately, the matrices symmetrically preconditioned by the BDS and RBIC(0) methods consistently require more than the 750 iterations I have allotted for calculating their eigenvalues. As a result, these counts may be incomplete, but should be reasonably close. The BDS method results in substantial improvement in the eigenvalue distribution as compared to the matrix without preconditioning. The RBIC(0) and IC(0) methods then each register moderate subsequent improvements. The IC(0) method, as would be expected, produces the "best" eigenvalue distribution of the three. It records the smallest spectral radius and causes the greatest number of eigenvalues to migrate into the lower interval.

Looking at Graph 4.9 - 4.11, we see that as the cost to transfer a piece of data between neighboring processors (ϕ) increases, the advantages of using the RBIC(0) factorization also increase. For $\phi = 10$, which may not be unrealistic for loosely connected processors, the RBIC(0) saves between 1500 and 60,000 time units over the IC(0) method. This advantage stems from the fact that the RBIC(0) method requires no data transfers to solve the system $z = C^{-1}r$, while the IC(0) method requires 2m data transfers.

Test Problem 1 (n=32)

Preconditioning Method	FACTOR Number of Elements in L	FACTOR Time	SOLVE Number of Iterations	SOLVE Time
None	0	0.0	92	2.98
BDS	992	0.03	70	2.77
RBIC(0)	1504	0.03	49	2.03
IC(0)	1984	0.02	46	1.92

Table 4.10 - Timing and convergence data pertaining to solving the given test problem, such that $||r|| \leq 10^{-6}$.

Preconditioning Method	Spectral Radius	Number of Eigenvalues in lower interval[1]	Number of Eigenvalues in upper interval[2]
None	8.664	10	9
BDS	2.281	30*	4
RBIC(0)	1.796	32*	6
IC(0)	1.591	46	3

* Number of Eigenvalues found after 750 iterations.

Table 4.11 - Data on the extreme Eigenvalues

Test Problem 2

Preconditioning Method	FACTOR Number of Elements in L	FACTOR Time	SOLVE Number of Iterations	SOLVE Time
None	0	0.0	99*	2.98
BDS	960	0.03	104	3.75
RBIC(0)	1456	0.03	75	2.86
IC(0)	1921	0.02	75	2.99

* $||r_{99}||$ = 0.105E-02

Table 4.12 - Timing and convergence data pertaining to solving the given test problem, such that $||r|| \leq 10^{-6}$.

Preconditioning Method	Spectral Radius	Number of Eigenvalues in lower interval[1]	Number of Eigenvalues in upper interval[2]
None	8.579	9	11
BDS	2.257	29*	5
RBIC(0)	1.798	35*	5
IC(0)	1.684	49	3

* Number of Eigenvalues found after 750 iterations.

Table 4.13 - Data on the extreme Eigenvalues.

Test Problem 3

Preconditioning Method	FACTOR Number of Elements in L	FACTOR Time	SOLVE Number of Iterations	SOLVE Time
None	0	0.0	99*	3.02
BDS	960	0.03	93	3.64
RBIC(0)	1456	0.02	68	2.60
IC(0)	1921	0.02	66	2.66

* $||r_{99}|| = 0.288E-02$

Table 4.14 - Timing and convergence data pertaining to solving the given test problem, such that $||r|| \leq 10^{-6}$.

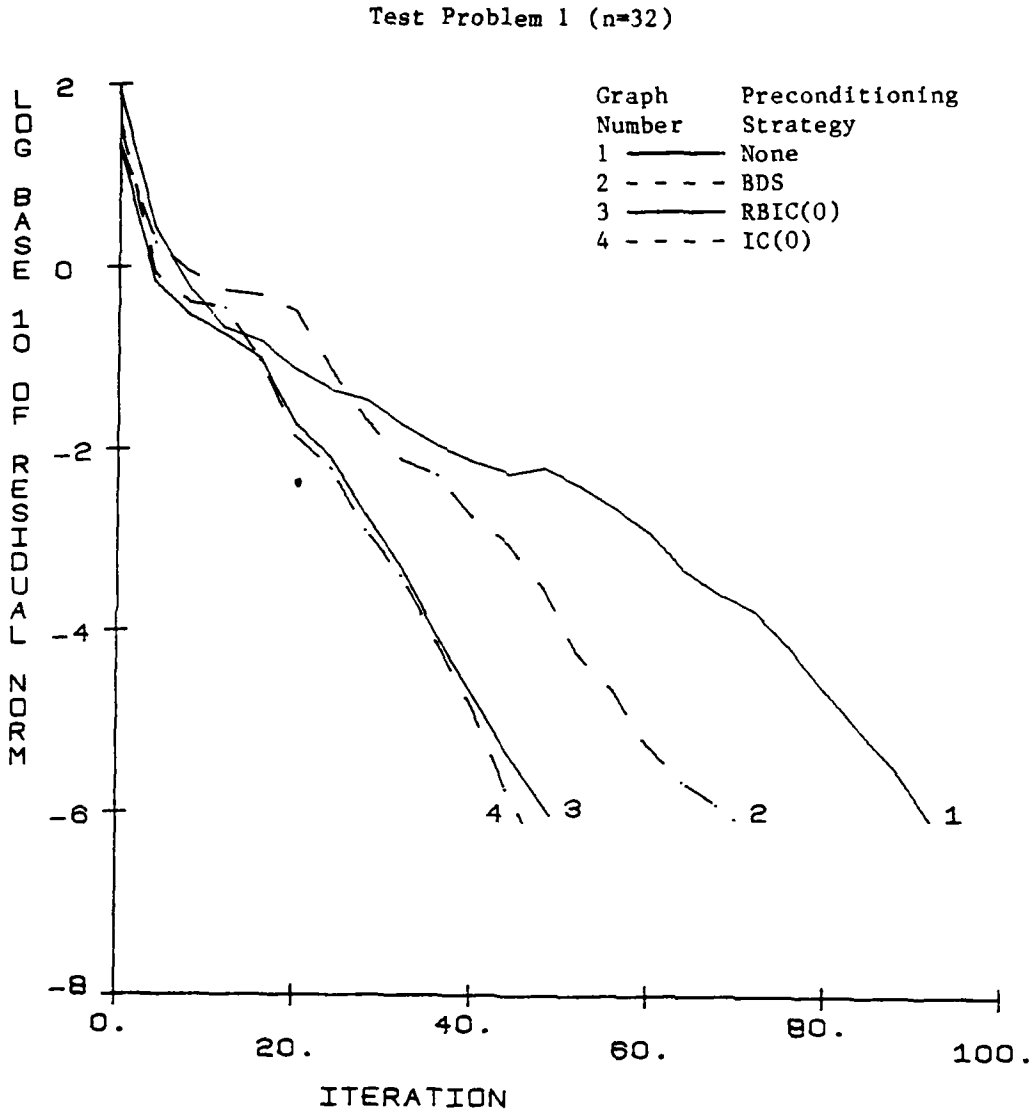
Preconditioning Method	Spectral Radius	Number of Eigenvalues in lower interval[1]	Number of Eigenvalues in upper interval[2]
None	22.977	4	1
BDS	2.236	31*	7
RBIC(0)	1.903	31*	5
IC(0)	1.634	49	6

* Number of Eigenvalues found after 750 iterations.

Table 4.15 - Data on the extreme Eigenvalues.

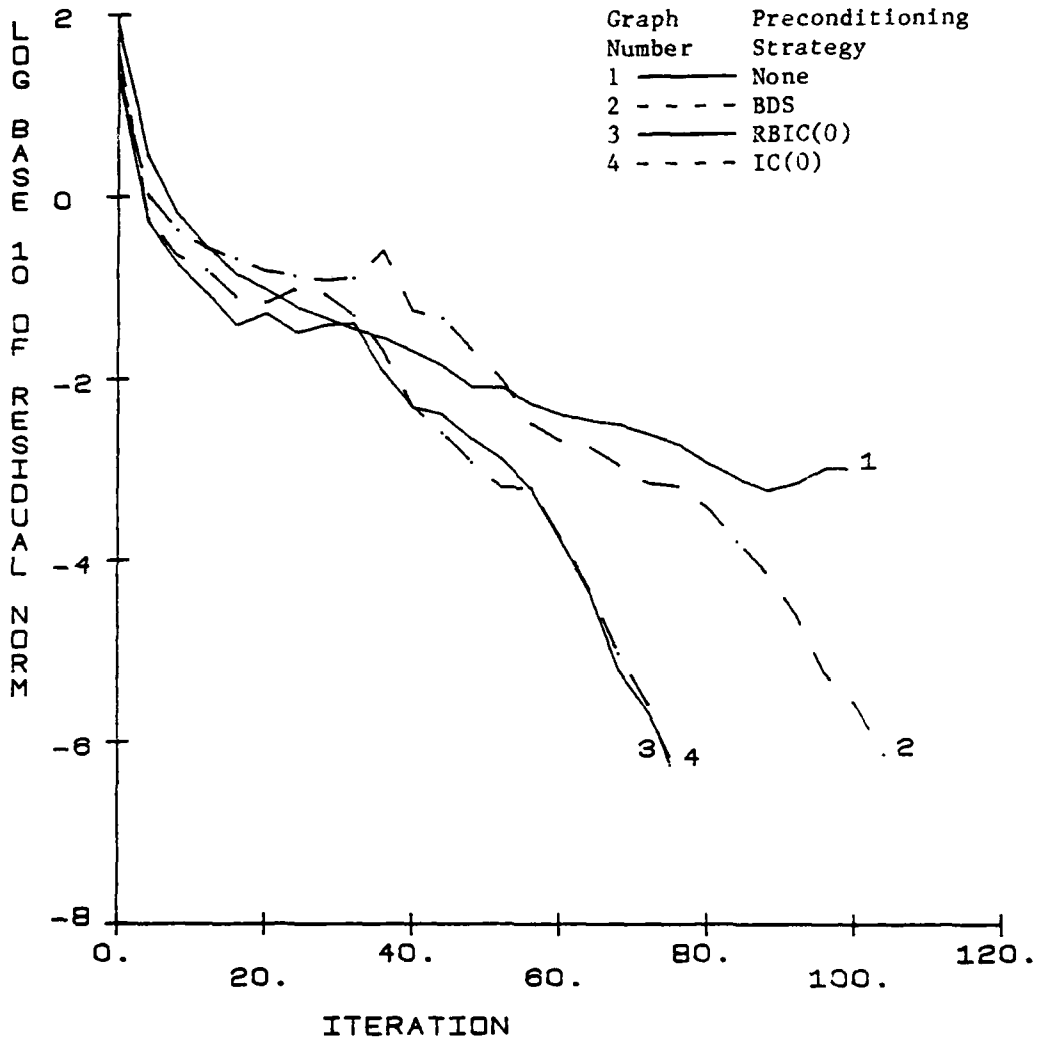
[1] - lower interval defined as [0.0,1.2]

[2] - upper interval defined as $[0.8\rho, \rho]$, where ρ = spectral radius.



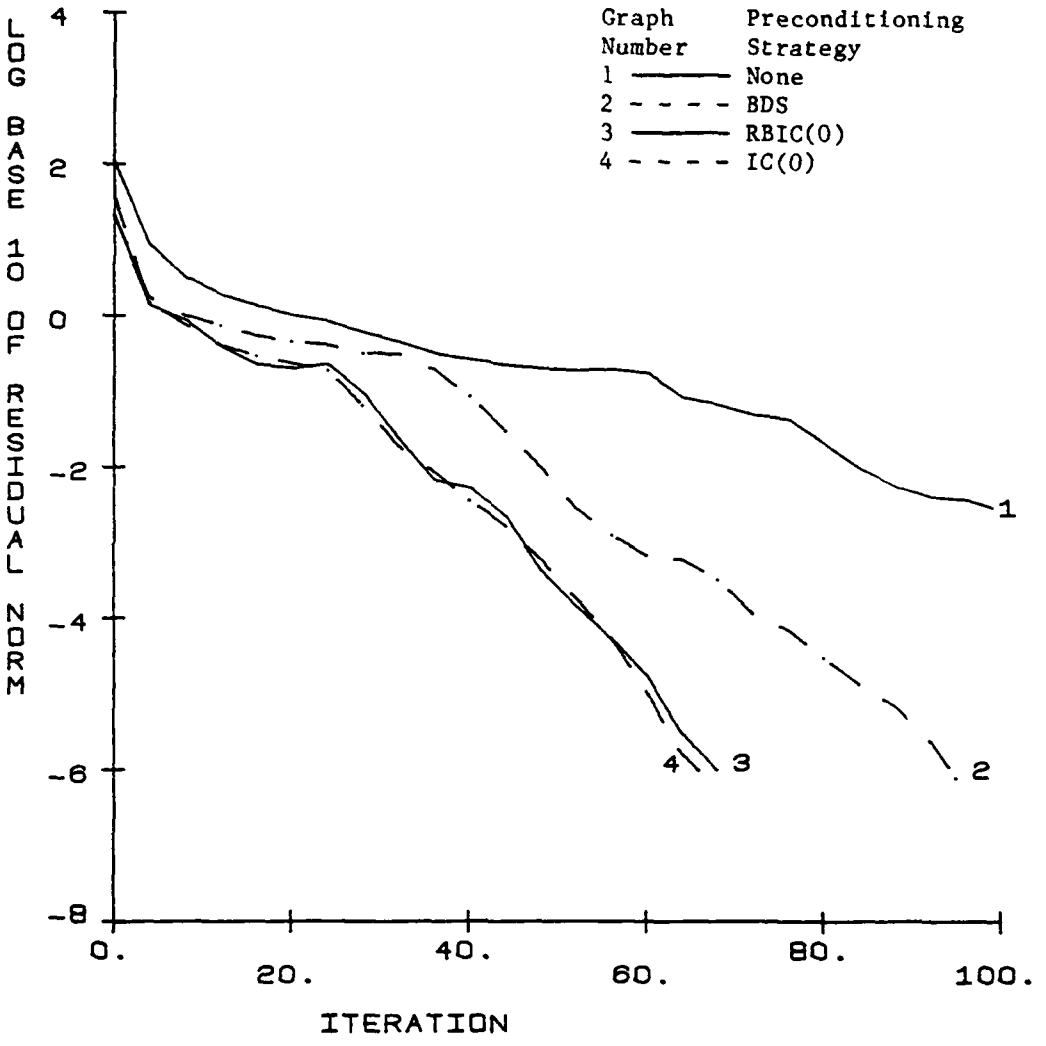
Graph 4.6 - The log base 10 of the norm of the residual as a function of the iteration number.

Test Problem 2

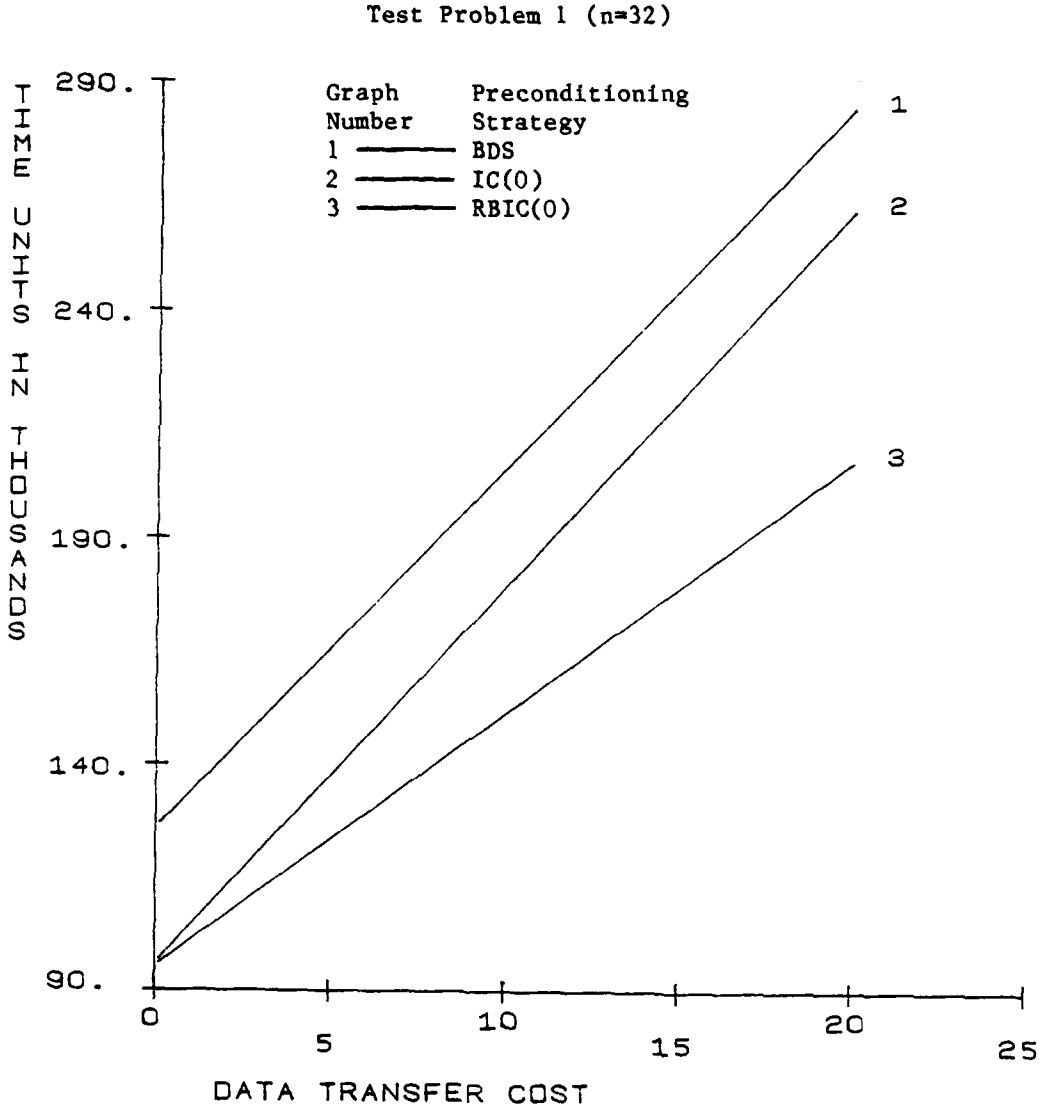


Graph 4.7 - The log base 10 of the norm of the residual as a function of the iteration number.

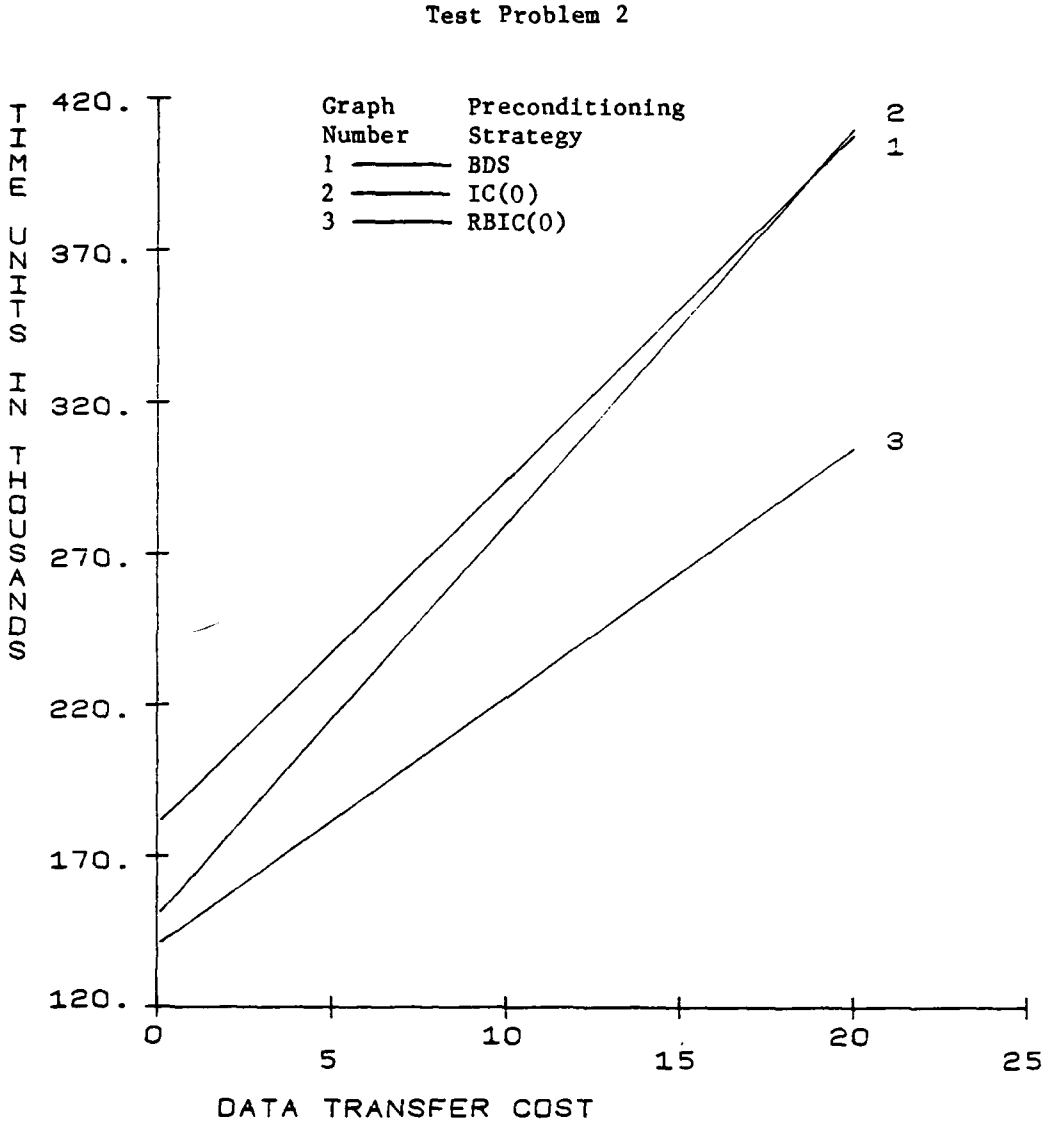
Test Problem 3



Graph 4.8 - The log base 10 of the norm of the residual as a function of the iteration number.

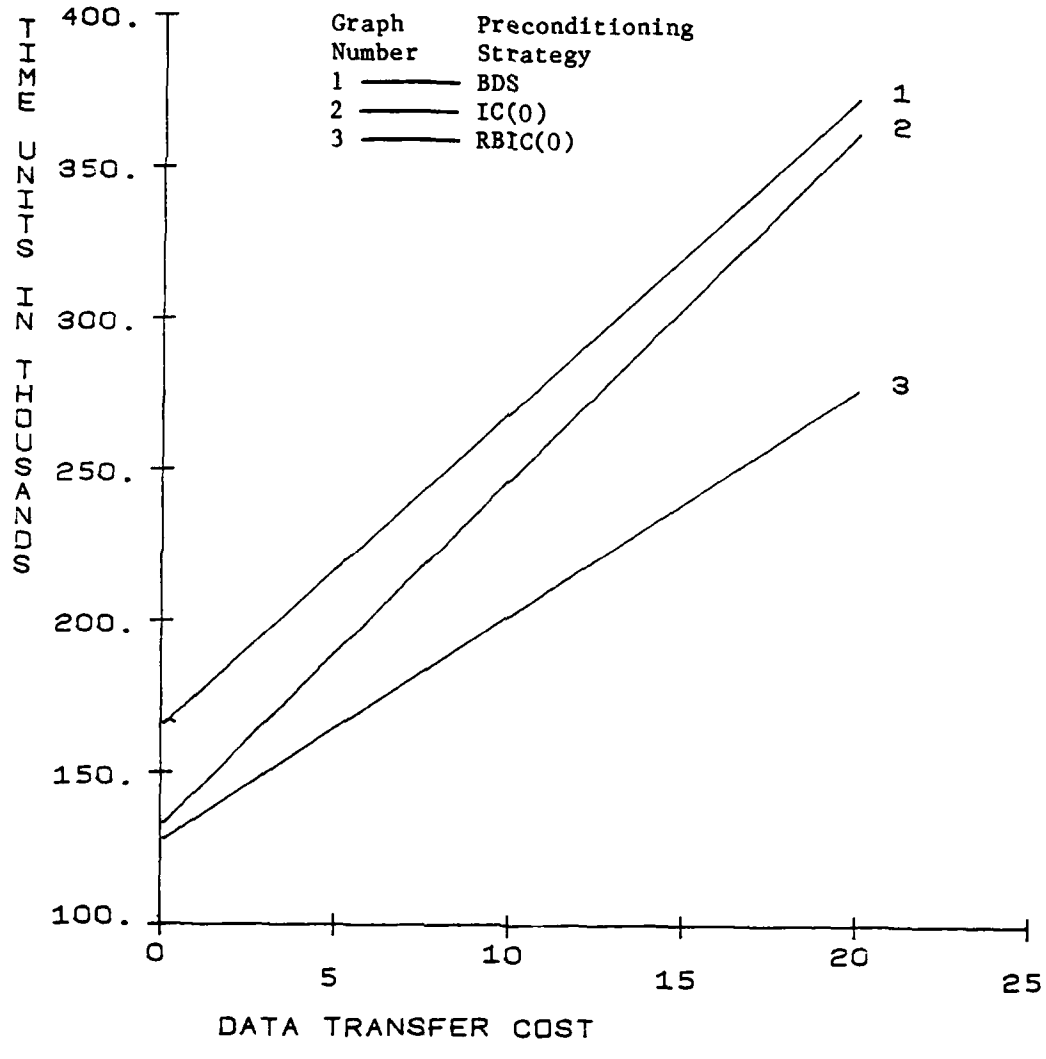


Graph 4.9 - Number of time units required to solve the given test problem vs. the cost in time units to transfer one piece of data between two processors.



Graph 4.10 - Number of time units required to solve the given test Problem vs. the cost in time units to transfer one piece of data between two processors.

Test Problem 3



Graph 4.11 - Number of time units required to solve the given test problem vs. the cost in time units to transfer one piece of data between two processors.

5. Conclusions

As we have seen, only a limited number of our original preconditioning strategies proved suitable for implementation on our multiprocessor. The DS, BDS, and RBIC(0) methods proved acceptable no matter which grid point ordering scheme was used. The IC(0) method, on the other hand, was only feasible when teamed with point red/black or line red/black matrices. When point red/black matrices were used, the IC(0) factorization could be performed without any interprocessor communications.

The numerical experiments showed that, for our given test problems of order ~1000, the RBIC(0) method, in most cases, was more efficient than the IC(0) method. This was especially true when viewed from the standpoint of our hypothetical multiprocessor. For values of $\phi >> 1$, the RBIC(0) method was substantially faster.

While I realize that these few test results do not prove that the RBIC(0) method is a superior method in all cases, they do indicate that the RBIC(0) method could be an efficient tool for preconditioning on a multiprocessor. More testing is needed to identify the scope of its potential.

Appendices

Appendix A

Grid point ordering schemes

Natural Ordering for n=6

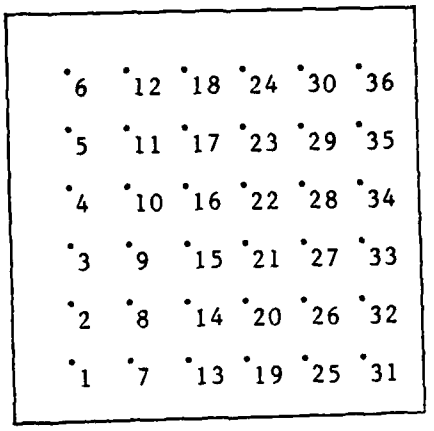


Figure A1

Point Red/Black Ordering for n=6

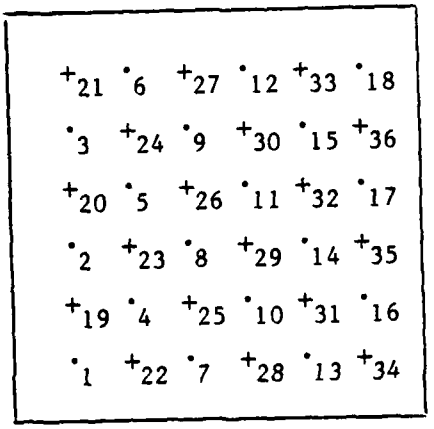


Figure A2

Line Red/Black Ordering for n=6

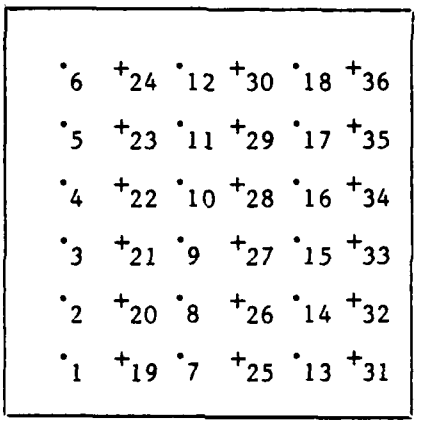


Figure A3

Two Line Red/Black Ordering for n=6

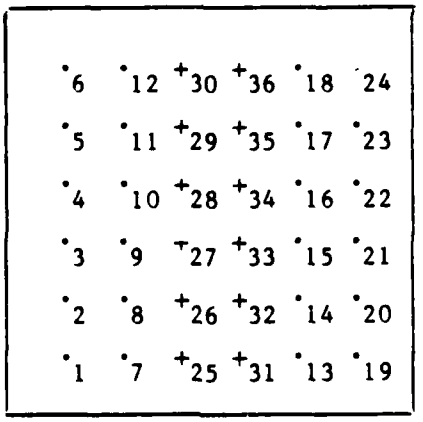


Figure A4

Non-zero Structure of Matrix with Natural Ordering

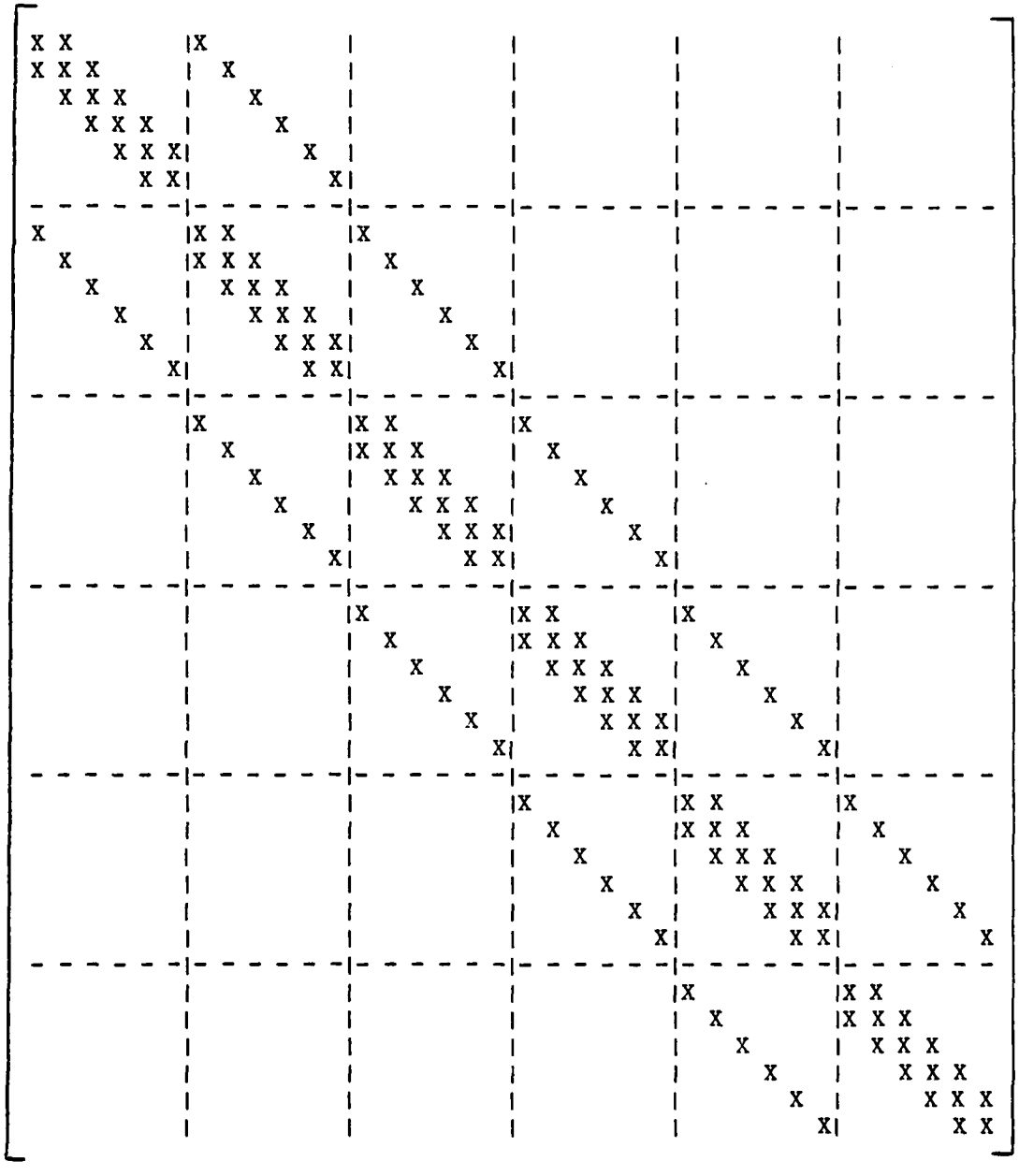


Figure A5

Non-zero Structure of Matrix with Point Red/Black Ordering

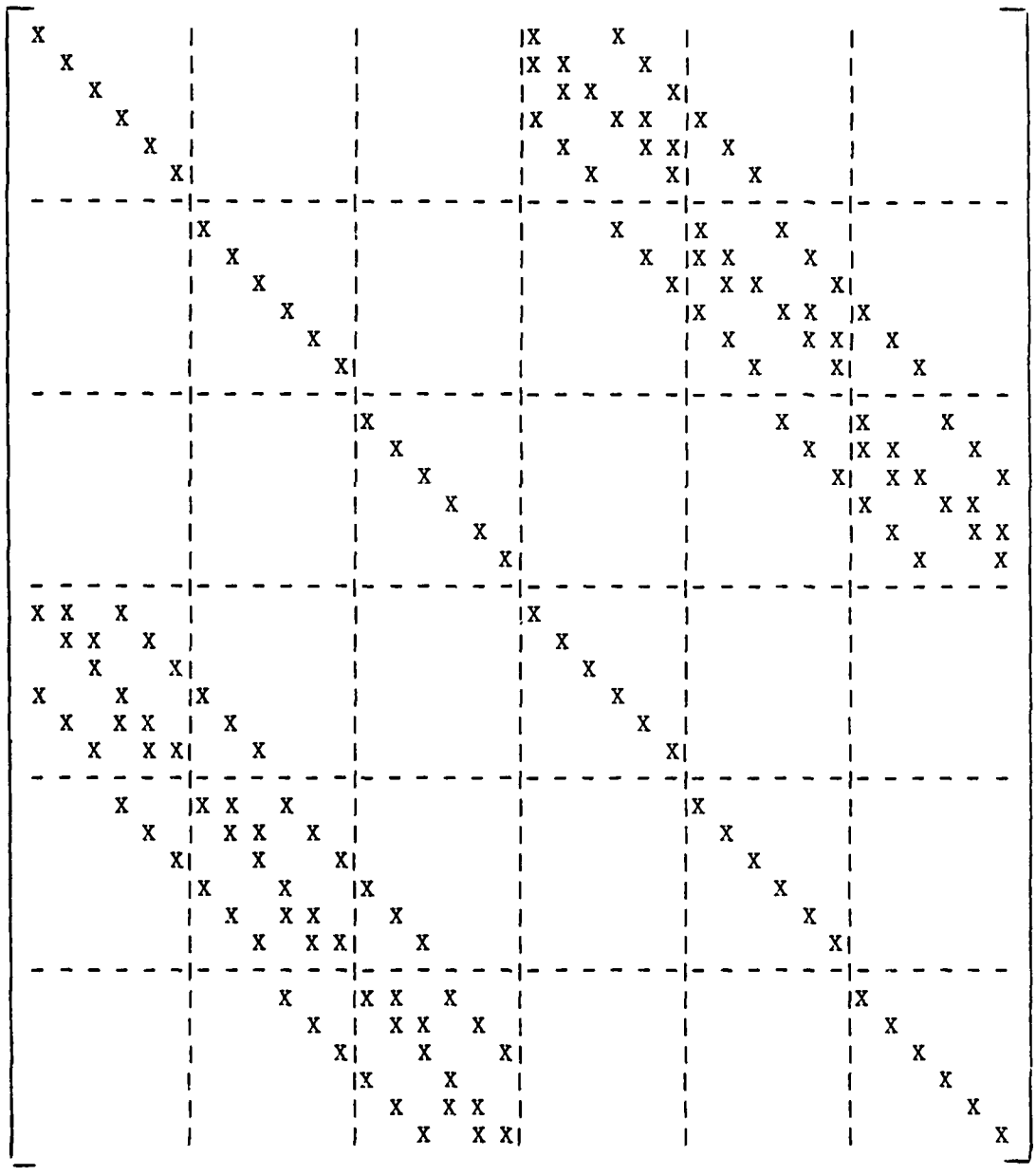


Figure A6

Non-zero Structure of Matrix with Line Red/Black Ordering

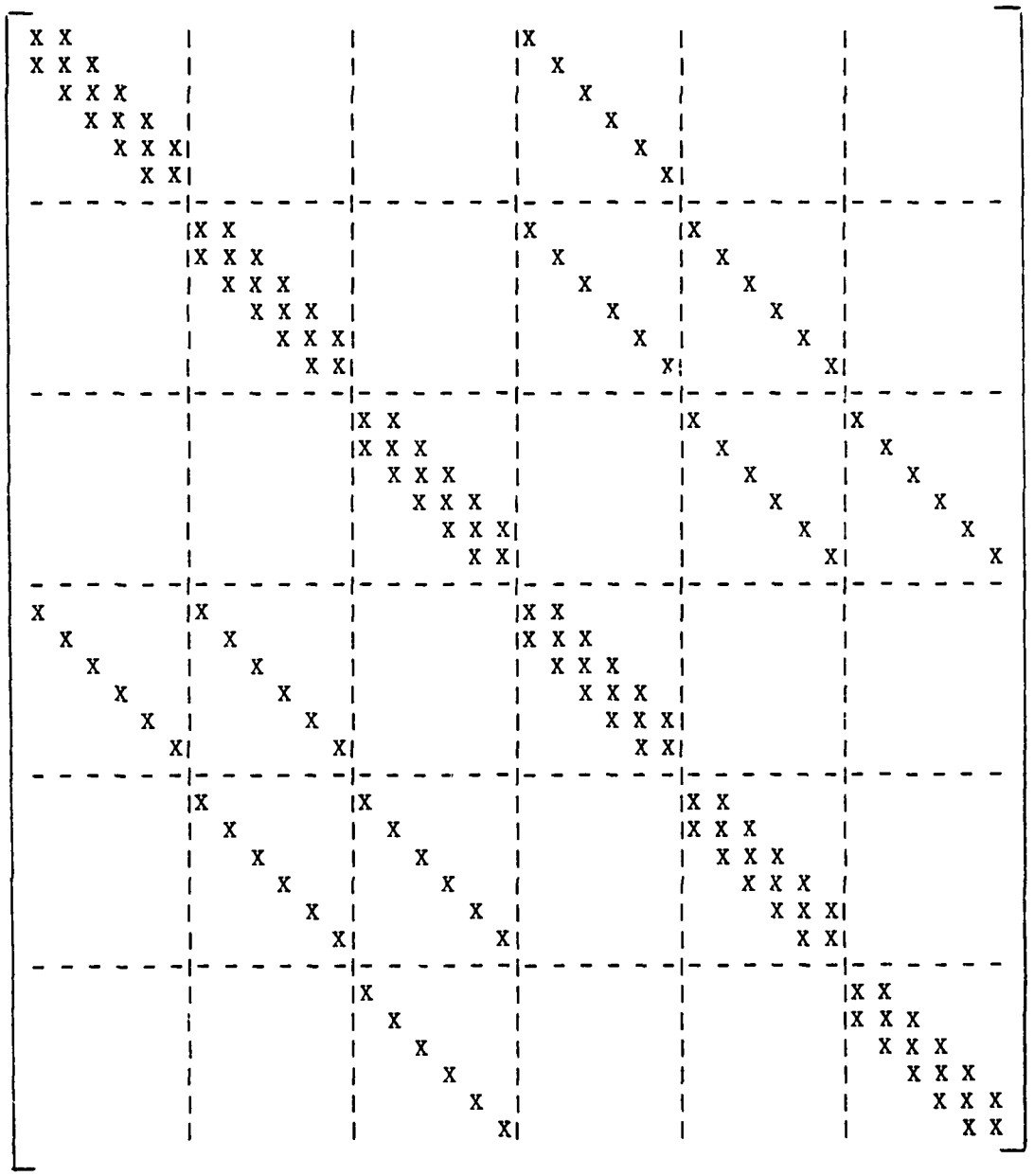


Figure A7

Non-zero Structure of Matrix with 2-line Red/Black Ordering

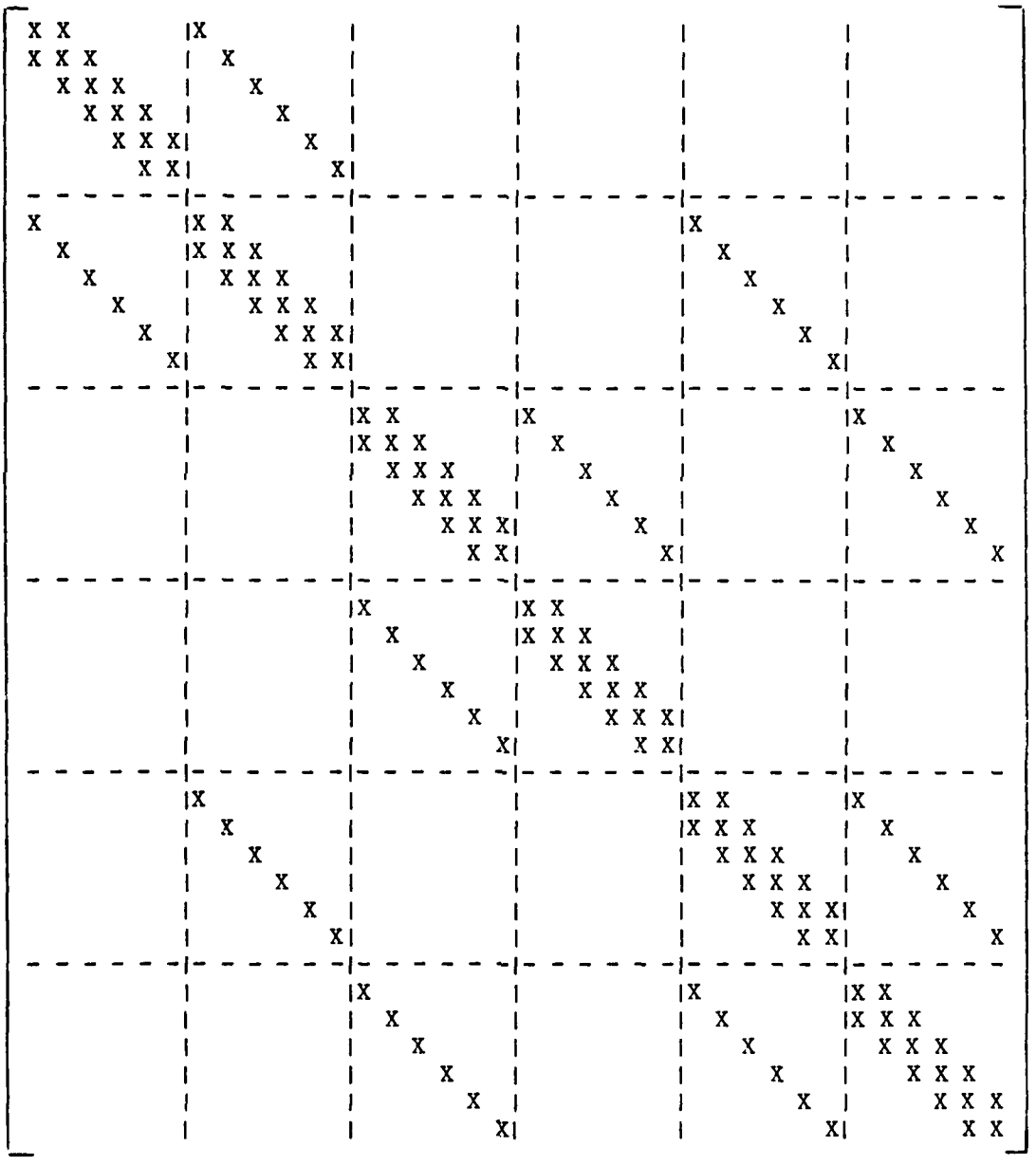


Figure A8

Appendix B

Matrix block structures

Appendix B shows the block structure of the matrices associated with the four grid point ordering schemes defined in Appendix A. I assume discretization took place on a n×m grid, with n being even.

Natural Ordering

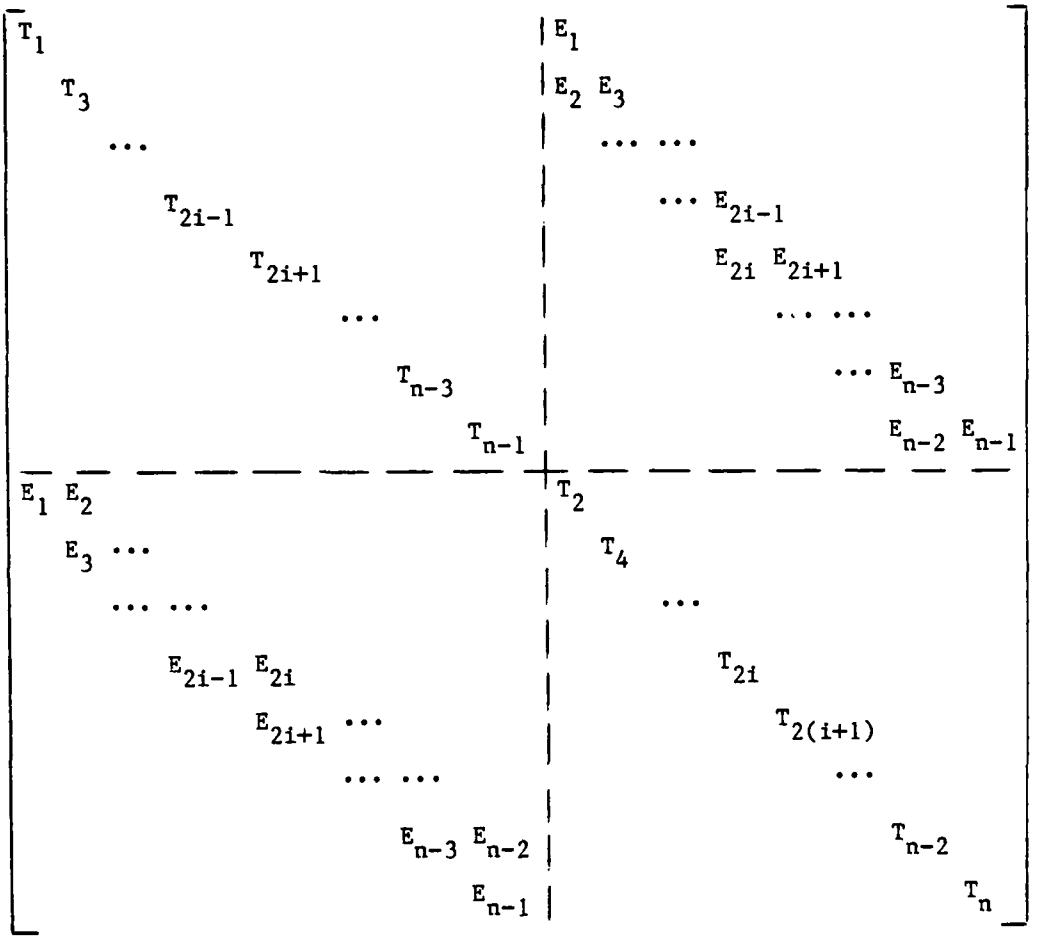
$$\begin{bmatrix}
T_1 & E_1 & & & & & & \\
E_1 & T_2 & E_2 & & & & & \\
 & \cdots & \cdots & \cdots & & & & \\
 & & E_{i-1} & T_i & E_i & & & \\
 & & & E_i & T_{i+1} & E_{i+1} & & \\
 & & & & E_{i+1} & T_{i+2} & E_{i+2} & \\
 & & & & & \cdots & \cdots & \cdots \\
 & & & & & & E_{n-2} & T_{n-1} & E_{n-1} \\
 & & & & & & & E_{n-1} & T_n
\end{bmatrix}$$

where E_i's are diagonal matrices of order m and

T_i's are tri-diagonal matrices of order m.

Figure B1

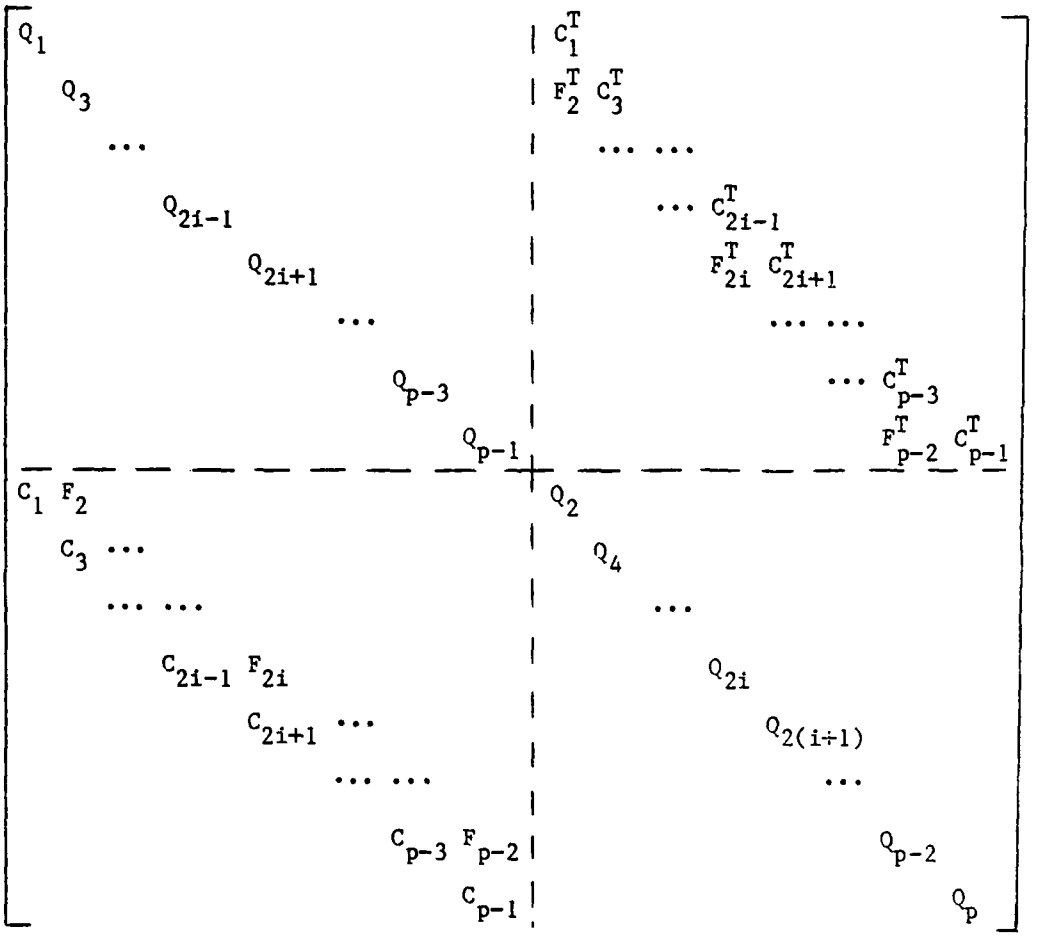
Line Red/Black Ordering



where T_i and E_i are the same as those used in figure B1

Figure B2

2-line Red/Black Ordering



where $k = n/2$ and $p = 2(\lceil k/2 \rceil)$

$$Q_i = \begin{vmatrix} T_{2i-1} & E_{2i-1} \\ E_{2i-1} & T_{2i} \end{vmatrix} \quad C_i = \begin{vmatrix} 0 & E_{2i} \\ 0 & 0 \end{vmatrix} \quad F_i = \begin{vmatrix} 0 & 0 \\ E_{2i} & 0 \end{vmatrix}$$

where T_i and E_i are the same as those used in figure B1.

If $p \neq k$, ignore last row and column.

Figure B3

Relating the block structure of the point red/black matrix to that of the naturally ordered matrix is not as easy as with the line red/black matrix and the 2-line red/black matrix. The integrity of the T_i and E_i blocks is not maintained during the reordering. A relationship does exist between the two, but not at the block level. We find that the point red/black matrix (A') and the naturally ordered matrix (A) are related such that

$$A' = P^T A P$$

where P is the permutation matrix

$$P = [P_1, P_2, \cdots, P_n; Q_1, Q_2, \cdots, Q_n],$$

in which for k = 1, 2, ···, n/2

$$P_{2k-1} = [e_{j(k)}, e_{j(k)+2}, e_{j(k)+4}, \cdots, e_{j(k)+m-2}],$$

$$Q_{2k-1} = [e_{j(k)+1}, e_{j(k)+3}, \cdots, e_{j(k)+m-1}],$$

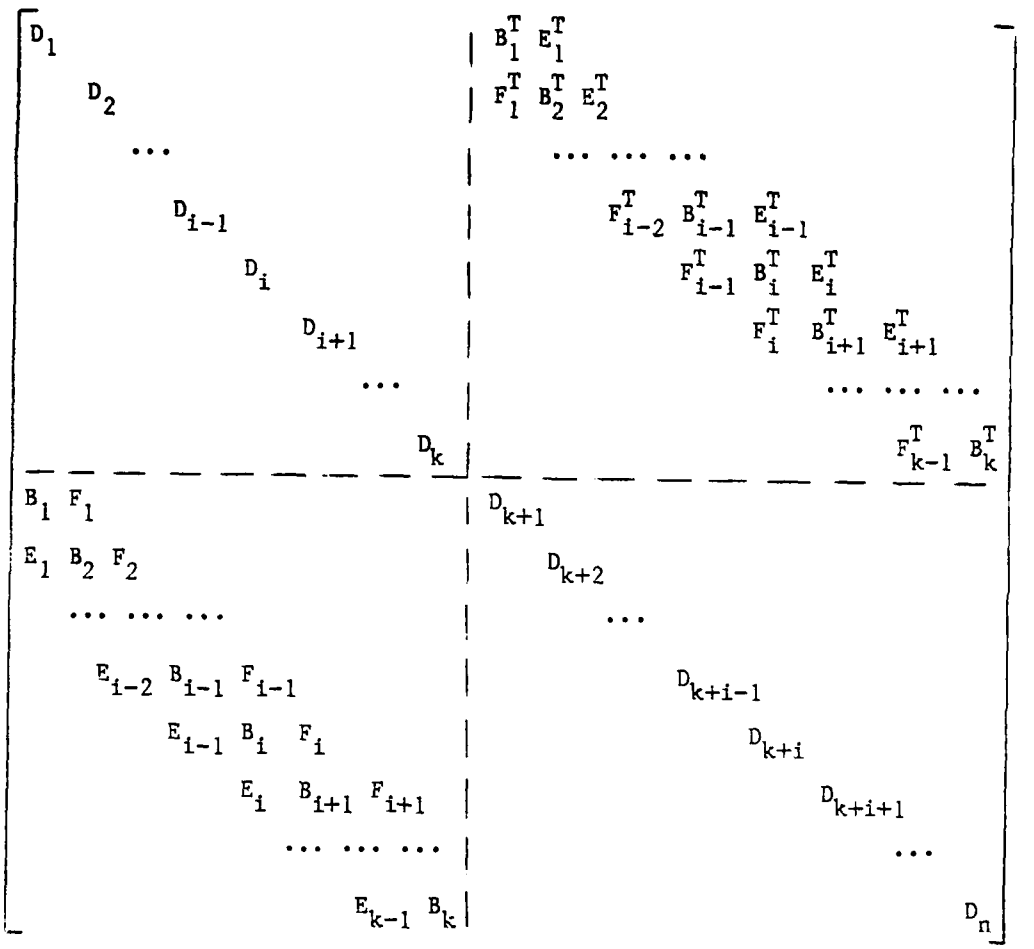
$$P_{2k} = [e_{1(k)}, e_{1(k)+2}, \cdots, e_{1(k)+m-2}],$$

$$Q_{2k} = [e_{1(k)-1}, e_{1(k)+1}, \cdots, e_{1(k)+m-3}],$$

with $j(k) = 2(k-1)m+1$ and $1(k) = j(k)+m+1$.

Figure B4 outlines the block structure for a point red/black matrix. The blocks here are different from those found in figures B1 - B3.

Point Red/Black Ordering



where $k = n/2$ and

$$B_i = \begin{vmatrix} B_{i1} & G_{i1} \\ G_{i2} & B_{i2} \end{vmatrix} \quad D_i = \begin{vmatrix} H_{i1} & 0 \\ 0 & H_{i2} \end{vmatrix} \quad E_i = \begin{vmatrix} 0 & E_{i1} \\ 0 & 0 \end{vmatrix} \quad F_i = \begin{vmatrix} 0 & 0 \\ F_{i2} & 0 \end{vmatrix}$$

with H_i, E_{i1}, F_{i2} and G_i being diagonal matrices of order m/2

and B_{i1} and B_{i2} being upper and lower bi-diagonal matrices of order m/2

Figure B4

Appendix C

User input parameters

Appendix C outlines the combinations of grid point ordering schemes and preconditioning strategies to be examined during phase I. The parameters and functions required by subroutine FACTOR to generate each of the combinations are defined. The abbreviations used to describe the various preconditioning strategies are defined in section 4.3.

Natural Ordering (NTYPE = 0)

Preconditioning Strategy	OPTION vector 1	2	3	4	5	6	C	Functions EUSE	FILL
None	-	-	-	-	-	1	-	-	-
DS	0	0	0	1	0	0	-	EUSE1	FILL1
BDS	0	0	0	1	0	0	-	EUSE2	FILL1
IC(0)	0	0	0	0	0	0	-	-	FILL1
IC(1)	0	0	0	0	0	0	-	-	FILL2
IC(3)	0	0	0	0	0	0	-	-	FILL3
MIC(0)	0	0	0	0	1	0	-	-	FILL1
HARWELL(10^{-2})	1	1	0	0	1	0	10^{-2}	-	-
HARWELL(0)	1	1	0	0	1	0	0.0	-	-
MICD(10^{-2})	0	1	0	0	1	0	10^{-2}	-	-
MICD(0)	0	1	0	0	1	0	0.0	-	-

Table C1

Line Red/Black Ordering (NTYPE = 1)

Precondtitioning	OPTION vector							Functions	
Strategy	1	2	3	4	5	6	C	EUSE	FILL
BDS	0	0	0	1	0	0	-	EUSE2	FILL1
IC(0)	0	0	0	0	0	-	-	FILL1	
HARWELL(10^{-2})	1	1	0	0	1	0	10^{-2}	-	-
HARWELL(0)	1	1	0	0	1	0	0.0	-	-
MICD(10^{-2})	0	1	0	0	1	0	10^{-2}	-	-
MICD(0)	0	1	0	0	1	0	0.0	-	-
RBIC(0)	0	0	0	1	0	0	-	EUSE3	FILL1
MIC(0)	0	0	0	0	1	0	-	-	FILL1

Table C2

Point Red/Black Ordering (NTYPE = 2)

Preconditioning Strategy	OPTION vector						C	Functions	
	1	2	3	4	5	6		EUSE	FILL
DS	0	0	0	1	0	0	-	EUSE1	FILL1
IC(0)	0	0	0	0	0	0	-	-	FILL1
HARWELL(10^{-2})	1	1	0	0	1	0	10^{-2}	-	-
HARWELL(0)	1	1	0	0	1	0	0.0	-	-
MICD(10^{-2})	0	1	0	0	1	0	10^{-2}	-	-
MICD(0)	0	1	0	0	1	0	0.0	-	-
RBIC(0)	0	0	0	1	0	0	-	EUSE4	FILL1
MIC(0)	0	0	0	0	1	0	-	-	FILL1

Table C3

2 Line Red/Black Ordering (NTYPE = 3)

Precondtitioning	OPTION vector							Functions	
Strategy	1	2	3	4	5	6	C	EUSE	FILL
BDS	0	0	0	1	0	0	-	EUSE2	FILL1
IC(0)	0	0	0	0	0	0	-	-	FILL1
MIC(0)	0	0	0	0	1	0	-	-	FILL1
HARWELL(10^{-2})	1	1	0	0	1	0	10^{-2}	-	-
HARWELL(0)	1	1	0	0	1	0	0.0	-	-
MICD(10^{-2})	0	1	0	0	1	0	10^{-2}	-	-
MICD(0)	0	1	0	0	1	0	0.0	-	-
RBIC(0)	0	0	0	1	0	0	-	EUSE5	FILL1
RBIC(3)	0	0	0	1	0	0	-	EUSE5	FILL3

Table C4

Definitions for parameters used in Tables C1 - C4.

OPTION(1) = 0 - Natural order factorization
1 - Minimum degree factorization
OPTION(2) = 0 - Function FILL used to control fill-ins
1 - Drop tolerance C used to control fill-ins
OPTION(3) = 0 - No diagonal scaling prior to factorization
1 - Diagonal elements scaled by 1+ABS(C)/N prior to factorization
OPTION(4) = 0 - All matrix elements used in calculating the incomplete factorization
1 - Function EUSE determines which matrix elements to use in calculating the incomplete factorization
OPTION(5) = 0 - No diagonal modification
1 - Diagonal modification performed
OPTION(6) = 0 - Calculate the desired preconditioning matrix
1 - Bypass calculating the preconditioining matrix

C - Drop tolerance used when OPTION(2) is in affect

EUSE - Function used to determine which elements of matrix A are to be used in calculating the incomplete factorization

FILL - Function used to determine which fill-ins to keep during the incomplete factorization

Appendix D

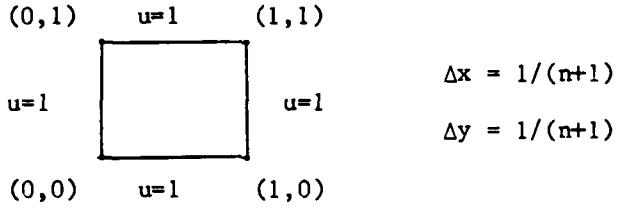
Definition of test problems.

Test Problem 1

Laplace Equation

$$-\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} = 0$$

over the unit square with Dirichlet boundary conditions:



$\Delta x = 1/(n+1)$

$\Delta y = 1/(n+1)$

Phase I

n=8 m=8

Matrix A of order 64

Phase III

n=32 m=32

Matrix A of order 1024

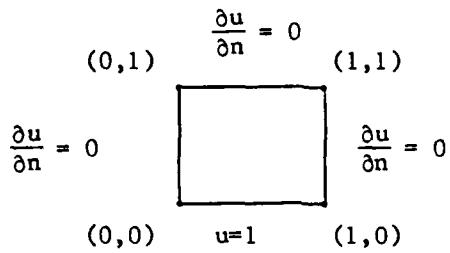
Matrix A will be a positive definite M-matrix.

Test Problem 2

Laplace Equation

$$-\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} = 0$$

over the unit square with boundary conditions:



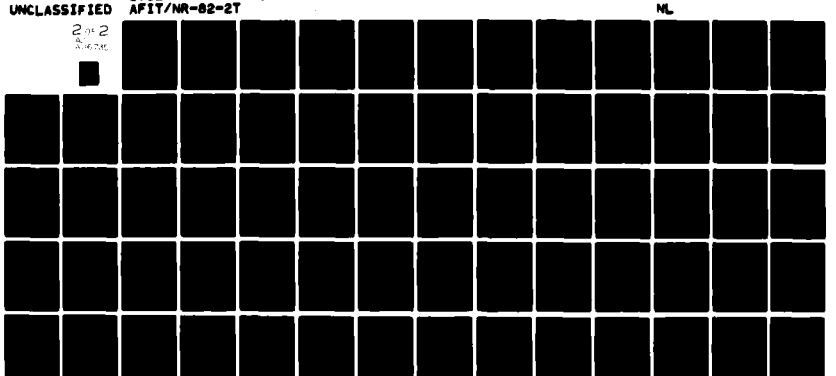
$\Delta x = 1/31 \qquad \Delta y = 1/31$

$n=32 \qquad m=31$

Matrix A is of order 992

Matrix A will be a positive definite M-matrix.

AD-A116 735 AIR FORCE INST OF TECH WRIGHT-PATTERSON AFB OH F/G 12/1
PRECONDITIONING STRATEGIES FOR SOLVING ELLIPTIC DIFFERENCE EQUA--ETC(U)
1982 C K TAFT
UNCLASSIFIED AFIT/NR-82-2T NL



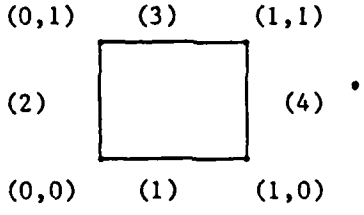
END
DATE FILMED
7-82
DTIC

Test Problem 3

$$-\frac{\partial}{\partial x}((x^2 + y^2 + 1)\frac{\partial}{\partial x}u) - \frac{\partial}{\partial y}(e^{xy}\frac{\partial}{\partial y}u) + u = f(x,y)$$

$$f(x,y) = e^{x^2y}(1 - (4x^4y^2 + 4x^2y^4 + 2x^2y^2 + 6x^2y + 2y^3 + 2y) - (x^4 + x^3)e^{xy})$$

over the unit square with boundary conditions



(1) $u = 1$

(2) $\frac{\partial u}{\partial n} = 0$

(3) $u + \frac{\partial u}{\partial n} = e^{x^2}(1 + x^2)$

(4) $2\frac{\partial u}{\partial n} = 4ye^{y}$

with $\Delta x = 1/31$ $\Delta y = 1/31$

$n=32$ $m=31$

Matrix A is of order 992

Matrix A will be positive definite, but not an M-matrix.

Appendix E

Cost of Conjugate Gradient Algorithm

Outlines the number of arithmetic operations and data transfers required by each step of our preconditioned conjugate gradient algorithm if implemented on our multiprocessor. I assume that the system of equations being solved is of order nm, where n is even, and that our multiprocessor consists of n/2 processors as arranged in figure 1.1.

	Arithmetic Operations	Interprocessor Data Transfers
Preprocessing factorization	*	*
CG Algorithm		
$x_0 = C^{-1}b$	*	*
$r = Ax_0 - b$	22m-8	2m
$(r^Tr)^{1/2}$	$4\frac{1}{2}m$	m/2
$g = C^{-1}r$	*	*
$e = -g$	0	0
$\delta_0 = r^Tg$	$4\frac{1}{2}m$	m/2
Each CG Iteration		
$f = Ae$	20m-8	2m
$\lambda = \delta_0/e^Tf$	$4\frac{1}{2}m$	m/2
$x = x + \lambda e$	4m	0
$r = r + \lambda f$	4m	0
$(r^Tr)^{1/2}$	$4\frac{1}{2}m$	m/2
$g = C^{-1}r$	*	*
$\delta_1 = r^Tg$	$4\frac{1}{2}m$	m/2
$\beta = \delta_1/\delta_0$	1	0
$\delta_0 = \delta_1$	0	0
$e = -g + \beta e$	4m	0

Table E1 - Cost breakdown of each step of a preconditioned conjugate gradient algorithm as implemented on our multiprocessor.

Preconditioning	Factorization		$g = C^{-1}r$	
Method	Arith. Ops.	Comm.	Arith. Ops.	Comm
BDS	6m	0	10m	0
IC(0)	13m	0	18m	2m
RBIC(0)	9m	0	14m	0

Table E2 - Cost breakdown of the preconditioning method dependent items from Table E1 for the preconditioning methods considered during Phase III.

Preconditioning	Preprocessing		1 CG iteration	
Method	Arith. Ops.	Comm.	Arith. Ops.	Comm.
None	31m	3m	$45\frac{1}{2}$m	$3\frac{1}{2}$m
BDS	57m	3m	$55\frac{1}{2}$m	$3\frac{1}{2}$m
IC(0)	80m	7m	$63\frac{1}{2}$m	$5\frac{1}{2}$m
RBIC(0)	68m	3m	$59\frac{1}{2}$m	$3\frac{1}{2}$m

Table E3 - Outlines the costs associated with the preprocessing stage and each CG iteration for the preconditioning strategies considered during Phase III if implemented on our multiprocessor.

Appendix F

Program Listings

Hierarchy Phase I Software

PROG1

- GENA
  - NORDER
  - ISTORE
  - MA31E*
- FACTOR
  - EUSE
  - MA31C
    - MA31D*
    - FILL
- SOLVE
  - MA31F
    - MA31G*
    - MA31H

PROG2

- GENA
  - NORDER
  - ISTORE
  - MA31E*
- FACTOR
  - EUSE
  - MA31C
    - MA31D*
    - FILL
- GETEIG
  - EA14AD*
  - MA31G2
  - MA31H
  - MA31G1
  - DSCRPT*
  - DSCRP2*

Heirarchy Phase III Software

PROG1A/B/C/D	PROG2A/B/C/D
. GENA	. GENA
. . NORDER	. . NORDER
. . ISTORE	. . ISTORE
. . MA31E*	. . MA31E*
. ICCG0/BDIAG/RBIC0	. ICCG0/BDIAG/RBIC0
. SOLVE	. GETEG2
. . MA31F	. . EA14AD*
. . MA31G*	. . MA31G2
. . MA31H	. . MA31H
	. . MA31G1

* Program listings for these routines are not included. They maybe found in the following locations:

MA31D, MA31E and MA31G - Cyber Harwell library as part of the MA31A package.

EA14AD - Cyber Harwell library

DSCRPT and DSCRP2 - Cyber MSL library

```
      PROGRAM PROG1(INPUT,OUTPUT,MESS,TAPE4=INPUT,TAPE5=MESS,
     *TAPE6=OUTPUT)
C
C  SOLVE THE LINEAR SYSTEM OF EQUATIONS ARISING FROM
C  THE DISCRETIZATION FOR OUR MODEL PROBLEM USING A
C  PRECONDITIONED CONJUGATE GRADIENT ALGORITHM.
C
C  SUBROUTINE GENA
C  ---------------
C    PERFORMS THE DISCRETIZATION OF THE CURRENT PROBLEM.
C    THE USER SPECIFIED INPUT PARAMETER NTYPE DETERMINES
C    THE TYPE OF GRID POINT ORDERING SCHEME TO BE USED:
C       NTYPE = 0  -  NATURAL
C               1  -  LINE RED/BLACK
C               2  -  POINT RED/BLACK
C               3  -  2 LINE RED/BLACK
C
C  SUBROUTINE FACTOR
C  -----------------
C    CALCULATES THE PRECONDITIONING MATRIX BY INCOMPLETE
C    FACTORIZATION.  THE TYPE OF INCOMPLETE FACTORIZATION
C    DONE IS DETERMINED BY THE USER SPECIFIED OPTION VECTOR:
C        OPTION(1) = 0  -  NATURAL ORDER FACTORIZATION
C                    1  -  MINIMUM DEGREE FACTORIZATION
C        OPTION(2) = 0  -  FUNCTION FILL USED TO CONTROL FILL-INS
C                    1  -  DROP TOLERANCE C USED TO CONTROL
C                          FILL-INS
C        OPTION(3) = 0  -  NO DIAGONAL SCALING PRIOR TO
C                          FACTORIZTION
C                    1  -  DIAGONAL ELEMENTS SCALED BY 1+ABS(C)/N
C                          PRIOR TO FACTORIZATION
C        OPTION(4) = 0  -  ALL MATRIX ELEMENTS USED IN CALCULATING
C                          THE INCOMPLETE FACTORIZATION
C                    1  -  FUNCTION EUSE DETERMINES WHICH MATRIX
C                           ELEMENTS TO USE IN CALCULATING
C                          THE INCOMPLETE FACTORIZATION
C        OPTION(5) = 0  -  NO DIAGONAL MODIFICATION
C                    1  -  DIAGONAL MODIFICATION PERFORMED
C        OPTION(6) = 0  -  CALCULATE THE DESIRED PRECONDITIONING
C                          MATRIX
C                    1  -  BYPASS CALCULATING PRECONDITIONING MATRIX
C
C  SUBROUTINE SOLVE
C  ----------------
C    SOLVES THE LINEAR SYSTEM USING THE HARWELL MA31F
C    PRECONDITIONED CONJUGATE GRADIENT ALGORITHM.
C       MITS - MAXIMUN NUMBER OF ITERATIONS ATTEMPTED
C       EPS - DESIRED ACCRACY OF SOLUTION IN TERM OF
```

```
      C              THE NORM OF THE RESIDUAL
50    C
      C  FOR MORE DETAILS SEE THE INDIVIDUAL SUBROUTINES.
      C
            REAL A(650),B(64),W(64,3),W1(64,3)
            INTEGER INI(200),INJ(650),IK(64,4),IW(64,4),OPTION(6)
55    C
            COMMON/MA31I/DD,LP,MP
            COMMON/MA31J/LROW,LCOL,NCP,ND,IPD
            COMMON/MA31K/NURL,NUCL,NUAL
            COMMON/MCOMM3/OPTION
60          COMMON/MA31L/EPSTOL,U
            COMMON/MA31M/NI,NJ,NVERSN,NTYPE
            COMMON/MA31N/MITS,EPS1
      C
            EXTERNAL FILL,EUSE
65    C
            DATA DD,LP,MP/1.0,6,5/
            DATA EPSTOL,U/2.0E-6,1.0E2/
            DATA NI,NJ/8,8/
            DATA IAI,IAJ,NN/200,650,64/
70          DATA MITS,EPS1/50,1.0E-6/
      C
            ND=NN
      C
            READ(4,*) NTYPE,NVERSN
75          READ(4,*) (OPTION(I),I=1,6)
            READ(4,*) C
      C
            CALL GENA(NN,NZ,A,INI,INJ,IAI,IAJ,W,B,IK,IW)
      C
80          IF (OPTION(6).EQ.1) GO TO 5
      C
      C  PERFORM THE DESIRED FACTORIZATION
      C
            CALL FACTOR(NN,NZ,A,INI,INJ,IAI,IAJ,IK,IW,W,C,FILL,EUSE)
85          GO TO 15
       5    CONTINUE
      C
      C  NO PRECONDITIONING REQUESTED
      C  GENERATE IDENTITY MATRIX
90    C
            LROW=0
            DO 10 I=1,NN
            IK(I,1)=0
            IK(I,2)=I
95          W(I,2)=1.0
      10    CONTINUE
```

```
      15   CONTINUE
      C
      C  PERFORM THE PRECONDITIONED CONJUGATE GRADIENT ITERATION
100   C
           CALL SOLVE(NN,NZ,A,INI,INJ,IAI,IAJ,W,IK,B,W1)
      C
           END



           SUBROUTINE GENA(NN,NZ,A,INI,INJ,IAI,IAJ,D,B,IK,IW)
      C
      C*******************************************************
      C
 5    C  GENA1
      C  -----
      C
      C  PERFORMS THE DISCRETIZATION OF THE LAPLACE EQUATION
      C  OVER THE UNIT SQUARE WITH DIRICHLET BOUNDARY CONDITIONS
10    C  USING A NI X NJ GRID.
      C  IDENTIFIED AS PROBLEM 1 IN TEXT.
      C
      C*******************************************************
      C
15    C  INPUT PARAMETERS
      C  ----------------
      C
      C  NN - ORDER OF MATRIX A
      C  IAI - SIZE OF ARRAY INI
20    C  IAJ - SIZE OF ARRAYS INJ AND A
      C
      C  OUTPUT PARAMETERS
      C  -----------------
      C
25    C   NZ - NUMBER OF NON-ZERO ELEMENTS IN THE UPPER
      C        TRIANGULAR PORTION OF MATRIX A
      C   A - ARRAY CONTAINING THE NON-ZERO ELEMENTS IN
      C       THE UPPER TRIANGULAR PORTION OF MATRIX A
      C       IN ROW ORDER
30    C   INI/INJ - ARRAYS CONTAINING THE ROW/COLUMN
      C              INDICES OF THE CORRESPONDING ENTRY
      C              IN ARRAY A (IE. INI(I) AND INJ(I)
      C              CONTAIN THE ROW AND COLUMN INDEX
      C              FOR THE ENTRY IN A(I) )
35    C   D - ARRAY CONTAINING THE DIAGONAL ELEMENTS OF
      C       MATRIX A
      C   B - CONTAINS THE RESULTING RIGHTHAND SIDE
```

```
C   IK(I,1) - NUMBER OF ELEMENTS IN ARRAY A BELONGING
C             TO ROW I
C   IK(J,2) - NUMBER OF ELEMENTS IN ARRAY A BELONGING
C             TO COLUMN J
C   IW(I) - POINTS TO THE FIRST ELEMENT OF ROW I IN
C           ARRAY A
C
C  COMMCN BLOCK PARAMETERS
C  ----------------------
C
C  LROW,LCOL,NCP,IPD,DD - NOT USED
C  ND - ORDER OF MATRIX A
C  LP - OUTPUT FILE UNIT NUMBER
C  MP - MESSAGE FILE UNIT NUMBER
C  NI - NUMBER OF GRID POINTS IN THE X DIRECTION
C  NJ - NUMBER OF GRID POINTS IN THE Y DIRECTION
C  NVERSN - PROBLEM IDENTIFIER
C  NTYPE - DETERMINES GRID POINT ORDERING TO BE
C          USED. SEE NORDER FOR DETAILS
C
      REAL A(IAJ),B(NN),D(NN),ATYPE(4)
      INTEGER INI(IAI),INJ(IAJ),IK(NN,2),IW(NN)
C
      COMMON/MA31J/LROW,LCOL,NCP,ND,IPD
      COMMON/MA31I/DD,LP,MP
      COMMON/MA31M/NI,NJ,NVERSN,NTYPE
C
      DATA ATYPE/7HNATURAL,7HLINE RB,8HPOINT RB,8H2LINE RB/
      WRITE(MP,2)
    2 FORMAT(11H GENA START)
C
C  INITIALIZE DATA
C
      DO 5 I=1,ND
      IK(I,1)=0
      IK(I,2)=0
      IW(I)=0
    5 CONTINUE
C
      CALL TIME(AT)
      CALL DATE(AD)
      CALL SECOND(TIM1)
C
      NNAT=0
      NZ=0
C
C  PROCESS GRID POINTS IN NATURAL ORDER
C  PERFORMING THE DISCRETIZATION
```

```
      C
            DO 100 J=1,NJ
            DO 90 I=1,NI
            NNAT=NNAT+1
 90         N=NORDER(NTYPE,I,J,NNAT)
            D(N)=4.0
            B(N)=0.0
            IF ((I.EQ.1).OR.(I.EQ.NI)) B(N)=B(N)+1.0
            IF ((J.EQ.1).OR.(J.EQ.NJ)) B(N)=B(N)+1.0
 95   C
            IF (I.EQ.NI) GO TO 50
            NZ=NZ+1
            A(NZ)=-1.0
            NT=NORDER(NTYPE,I+1,J,NNAT+1)
100         CALL ISTORE(N,NT,INI,INJ,IAI,IK,ND,NZ)
      C
       50   CONTINUE
            IF (J.EQ.NJ) GO TO 90
            NZ=NZ+1
105         A(NZ)=-1.0
            NT=NORDER(NTYPE,I,J+1,NNAT+NI)
            CALL ISTORE(N,NT,INI,INJ,IAI,IK,ND,NZ)
      C
       90   CONTINUE
110    100  CONTINUE
      C
      C  INITIALIZE IW(I) TO POINT JUST BEYOND WHERE THE
      C  LAST COMPONENT OF ROW I WILL BE STORED
      C
115         KI=1
            DO 200 I=1,ND
            KI=KI+IK(I,1)
       200  IW(I)=KI
      C
120   C  REORDER BY ROWS USING IN-PLACE SORT ALGORITHM
      C
            CALL MA31E(INI,INJ,NZ,IW,ND,A)
      C
      C  REINITIALIZE IW(I) TO POINT TO THE BEGINNING OF ROW I
125   C
            KK=1
            DO 210 IR=1,ND
            IW(IR)=KK
       210  KK=KK+IK(IR,1)
130         DO 220 I=1,NZ
       220  INI(I)=IABS(INI(I))
      C
            CALL SECOND(TIM2)
```

```
      TIMD=TIM2-TIM1
C
C  OUTPUT STATISTICS
C
      WRITE(LP,250) TIMD
 250  FORMAT(13H GENA TIME = ,F6.3,4H SEC)
      WRITE(LP,260) NVERSN
 260  FORMAT(11H VERSION = ,I2)
      WRITE(LP,265) ATYPE(NTYPE+1)
 265  FORMAT(14H MATRIX A HAS ,A10,9H ORDERING)
      WRITE(LP,270) AD,AT
 270  FORMAT(18H DATE GENERATED = ,A10,A10)
      WRITE(LP,280) ND,NZ
 280  FORMAT(6H ND = ,I4,6H NZ = ,I4)
      WRITE(MP,290)
 290  FORMAT(9H GENA END)
C
      RETURN
      END
      SUBROUTINE ISTORE(N,NJ,INI,INJ,IAI,IK,NP,NZ)
C
      INTEGER INI(IAI),INJ(IAI),IK(NP,2)
C
C  SUBROUTINE USED TO UPDATE ROW AND COLUMN COUNTS
C
      IF (N.GT.NJ) GO TO 10
      INI(NZ)=N
      IK(N,1)=IK(N,1)+1
      INJ(NZ)=NJ
      IK(NJ,2)=IK(NJ,2)+1
      GO TO 20
 10   INI(NZ)=NJ
      IK(NJ,1)=IK(NJ,1)+1
      INJ(NZ)=N
      IK(N,2)=IK(N,2)+1
 20   CONTINUE
      RETURN
      END




      FUNCTION NORDER(NTYPE,I,J,N)
C
C  SUBROUTINE TO PERMUTE AN ELEMENT FROM NATURAL ORDERING TO
C  ONE OF THE OTHER ORDERING SCHEMES
C
C  NTYPE = 0  NATURAL ORDERING
```

```
C         = 1  LINE RED/BLACK ORDERING
C         = 2  POINT RED/BLACK ORDERING
C         = 3  2 LINE RED/BLACK ORDERING
C
      INTEGER PTRB,OFFST(4)
      COMMON/MA31M/NI,NJ,NVERSN,NTYP
      DATA OFFST/32,512,496,496/
      DATA NATURL,LINRB,PTRB,L2RB/0,1,2,3/
C
      NTEMP=N
C
      IF (NTYPE.EQ.NATURL) GO TO 100
C
      IMOD=MOD(I+1,2)
      JMOD=MOD(J+1,2)
C
C DETERMINE IF LINE RED-BLACK ORDERING REQUESTED
C
      IF (NTYPE.NE.LINRB) GO TO 20
      NTEMP=J+((I-1)/2)*NJ
      IF (IMOD.EQ.0) GO TO 15
      NTEMP=NTEMP+OFFST(NVERSN+1)
   15 CONTINUE
      GO TO 100
   20 CONTINUE
C
C  DETERMINE IF POINT RED-BLACK ORDERING REQUESTED
C
      IF (NTYPE.NE.PTRB) GO TO 30
      NTEMP=(N+1)/2
      IF (IMOD.EQ.JMOD) GO TO 25
      NTEMP=NTEMP+OFFST(NVERSN+1)
   25 CONTINUE
      GO TO 100
   30 CONTINUE
C
C  DETERMINE IF TWO LINE RED-BLACK ORDERING  REQUESTED
C
      NTEMP=J+IMOD*NJ+((I-1)/4)*NJ*2
      NIMOD=MOD((I+1)/2,2)
      IF (NIMOD.EQ.1) GO TO 100
      NTEMP=NTEMP+OFFST(NVERSN+1)
C
  100 CONTINUE
      NORDER=NTEMP
      RETURN
      END
```

```
      SUBROUTINE FACTOR(NN,NZA,A,INI,INJ,IAI,IAJ,IK,IW,
     *W,C,FILL,EUSE)
C
C  SUBROUTINE TO CALCULATE THE PRECONDITIONING MATRIX
C  USING THE MODIFIED HARWELL ROUTINE MA31C.  THIS
C  SUBROUTINE PERFORMS THE SAME FUNCTIONS AS THE
C  HARWELL ROUTINE MA31A.  SEE DESCRIPTION OF THE HARWELL
C  MA31 PACKAGE FOR MORE DETAILS.
C
      REAL A(IAJ),W(NN,3)
      INTEGER IK(NN,4),IW(NN,4),INI(IAI),INJ(IAJ),OPTION(6)
      LOGICAL FILL,EUSE
C
      COMMON/MA31I/DD,LP,MP
      COMMON/MA31J/LROW,LCOL,NCP,ND,IPD
      COMMON/MA31K/NURL,NUCL,NUAL
      COMMON/MCOMM3/OPTION
      COMMON/MA31M/NI,NJ,NVERSN,NTYPE
C
      CALL SECOND(TIM1)
C
      NZ=NZA
      NZP1=NZA+1
      IAJ1=IAJ-NZA
C
C  SAVE ROW INDEX FILE IK(K,1)
C
      DO 5 K=1,NN
    5 IK(K,4)=IK(K,1)
C
      IF (OPTION(4).EQ.0) GO TO 18
C
C  ELIMINATE THOSE ELEMENTS NOT TO BE USED IN THE
C  INCOMPLETE FACTORIZATION AS DETERMINED BY THE
C  FUNCTION EUSE.
C
      NZ1=NZ+1
      KK=NZ
      DO 12 K=1,NZ
      I=INI(K)
      J=INJ(K)
      IF (EUSE(I,J)) GO TO 10
      IK(I,1)=IK(I,1)-1
      IK(J,2)=IK(J,2)-1
      GO TO 12
   10 CONTINUE
      KK=KK+1
      A(KK)=A(K)
```

```
            INJ(KK)=J
 12         CONTINUE
C
C  REBUILD THE START OF ROW I FILE IW(I,1)
C
            KI=NZ1
            DO 14 K=1,ND
            IW(K,1)=KI
            KI=KI+IK(K,1)
 14         CONTINUE
C
            NZ=KK-NZA
            CALL SECOND(TIM2)
C
            IF (NZ.NE.0) GO TO 18
C
C  SPECIAL CASE OF DIAGONAL SCALING
C
            DO 15 I=1,ND
            W(I,2)=W(I,1)
            IK(I,2)=I
 15         CONTINUE
            LROW=0
            LCOL=0
            IFLAG=0
            GO TO 45
C
C  CONSTRUCT COLUMN FILE IW(I,2) TO POINT JUST BEYOND WHERE THE
C  LAST COMPONENT OF COLUMN I WILL BE STORED
C
 18         KJ=IAI-NZ+1
            DO 20 I=1,ND
            KJ=KJ+IK(I,2)
            IW(I,2)=KJ
 20         CONTINUE
C
C  CONSTRUCT COLUMN FILE IN HIGH ORDER PART OF INI
C
            DO 30 IR=1,ND
            KPP=IW(IR,1)
            KLL=KPP+IK(IR,1)-1
            IF (KPP.GT.KLL) GO TO 30
            DO 25 K=KPP,KLL
            J=INJ(K)
            KR=IW(J,2)-1
            IW(J,2)=KR
            INI(KR)=IR
 25         CONTINUE
```

```
 30   CONTINUE
C
C  TRANSFER INPUT MATRIX TO TAIL END OF ARRAY A
C  AND MODIFY INJ TO REFLECT THE MOVE
C

      NUAL=IAJ+1
      DO 40 II=1,ND
      I=ND-II+1
      W(I,2)=W(I,1)
      KP=IW(I,1)
      KL=KP+IK(I,1)-1
      IF (KP.GT.KL) GO TO 38
      DO 35 KK=KP,KL
      K=KP+KL-KK
      NUAL=NUAL-1
      A(NUAL)=A(K)
      INJ(NUAL)=INJ(K)
 35   CONTINUE
 38   IW(I,1)=NUAL-NZA
 40   CONTINUE
C
C  INITIALIZE COMMON MA31J AND MA31K VARIABLES
C
      LCOL=NZ
      LROW=NZ
      NURL=0
      NUCL=IW(1,2)
      NUAL=NUAL-NZA
      IFLAG=0
      NCP=0
C
      CALL SECOND(TIM2)
C
C  PERFORM THE FACTORIZATION
C
      CALL MA31C(ND,NZ,W(1,2),A(NZP1),INI,INJ(NZP1),
     1IAI,IAJ1,IK,IW,IW(1,3),W(1,3),IFLAG,C)
C
 45   CALL SECOND(TIM3)
C
C  RESTORE INI
C
      KP=1
      DO 56 I=1,ND
      KL=KP+IK(I,4)-1
      IF (KP.GT.KL) GO TO 56
      DO 55 K=KP,KL
```

```
      55    INI(K)=I
145   56    KP=KL+1
      C
      C OUTPUT STATISTICS ON THE FACTORIZATION
      C
            WRITE(LP,58)
150   58    FORMAT(25HORESULTS OF FACTORIZATION)
            WRITE(LP,60) (OPTION(I),I=1,6),C
      60    FORMAT(1HO,9HOPTION = 6I1,2X,4HC = ,F9.5)
            WRITE(LP,65) IFLAG
      65    FORMAT(9H IFLAG = ,I3)
155   C
      C  TPD - TIME REQUIRED TO PREPARE DATA ARRAYS
      C        PRIOR TO CALLING MA31C.
      C  TD - TIME REQUIRED BY MA31C TO PERFORM THE
      C       FACTORIZATION.
160   C  TDT - TOTAL TIME REQUIRED BY SUBROUTINE FACTOR.
      C
            TDT=TIM3-TIM1
            TPD=TIM2-TIM1
            TD=TIM3-TIM2
165   C
            WRITE(LP,70) TDT,TPD,TD
      70    FORMAT(7H TDT = ,F6.3,7H TPD = ,F6.3,6H TD = ,F6.3)
      C
            WRITE(LP,85) NTYPE,NVERN
170   85    FORMAT(9H NTYPE = ,I2,2X,10HVERSION = ,I2)
            WRITE(LP,90) LROW
      90    FORMAT(21HONUM ELEMENTS IN L = ,I4)
            WRITE(LP,100) ND,NZA
      100   FORMAT(6H ND = ,I3,7H NZA = ,I4)
175   C
      150   CONTINUE
            RETURN
            END
```

```
      LOGICAL FUNCTION EUSE(I,J)
C
C  EUSE1
C  -----
5  C
C  ELIMINATES ALL OFF-DIAGONAL ELEMENTS.
C  USED FOR DIAGONAL SCALING
C
      EUSE=.FALSE.
10    RETURN
      END
```

```
      LOGICAL FUNCTION EUSE(I,J)
C
C  EUSE 2
C  ------
5  C
C  USED DURING BLOCK DIAGONAL SCALING (BDS).
C  KEEPS ONLY THOSE ELEMENTS IN THE TRI-DIAGONAL
C  PORTION OF THE MATRIX A.
C
      EUSE=.FALSE.
10    IF (IABS(J-I).LE.1) EUSE=.TRUE.
      RETURN
      END
```

```
      LOGICAL FUNCTION EUSE(I,J)
C
C  EUSE3
C  -----
5  C
C  USED TO GENERATE THE LINE RED/BLACK REDUCED BLOCK FORMAT
C
      EUSE=.FALSE.
      ID=IABS(J-I)
10    IF ((ID.LE.1).OR.(ID.EQ.32)) EUSE=.TRUE.
      RETURN
      END
```

```
      LOGICAL FUNCTION EUSE(I,J)
C
C  EUSE4
C  -----
C
C  USED TO GENERATE THE POINT RED/BLACK
C  REDUCED BLOCK MATRIX.
C
      EUSE=.FALSE.
      MI=(I-1/8)+1
      MJ=((J-1)/8)+1
      MD=IABS(MJ-MI)
      IF (MD.EQ.4) EUSE=.TRUE.
      RETURN
      END



      LOGICAL FUNCTION EUSE(I,J)
C
C  EUSE5
C  -----
C
C  USED TO GENERATE THE 2 LINE RED/BLACK REDUCED BLOCK FORMAT
C
      EUSE=.FALSE.
      IF (IABS(J-I).LE.8) EUSE=.TRUE.
      RETURN
      END



      SUBROUTINE MA31C(N,NZ,D,A,INI,INJ,IAI,IAJ,IK,
     1IP,IW,W,IFLAG,C)
C
C  MA31C IS PART OF THE HARWELL MA31 PACKAGE.
C  SEE ROUTINE MA31A FOR DETAILS.
C  MODIFIED TO CALCULATE A WIDER VARIETY OF INCOMPLETE
C  CHOLESKY FACTORIZATIONS.
C
      EXTERNAL FILL
      REAL A(IAJ),W(N),D(N)
      INTEGER IP(N,2),OPTION(6)
      LOGICAL CHANGE,FILL
      INTEGER IK(N,3),IW(N,2),INI(IAI),INJ(IAJ)
      COMMON/MA31I/DD,LP,MP
```

```
      COMMON/MA31J/LROW,LCOL,NCP,ND,IPD
      COMMON/MA31K/NURL,NUCL,NUAL
      COMMON/MCOMM3/OPTION
      COMMON/MA31L/EPSTOL,U
C
C  OPTION DETERMINES HOW THE FACTORIZATION WILL BE DONE
C     OPTION(1) = 0  -  NATURAL ORDER FACTORIZATION
C               = 1  -  MINIMUM DEGREE FACTORIZATION
C     OPTION(2) = 0  -  FUNCTION FILL USED TO CONTROL FILL-INS
C               = 1  -  DROP TOLERANCE C USED TO CONTROL FILL-INS
C     OPTION(3) = 0  -  NO DIAGONAL SCALING USED
C               = 1  -  DIAGONAL ELEMENTS SCALED BY
C                       1+ABS(C)/FLOAT(N)
C     OPTION(4)      -  NOT USED HERE
C     OPTION(5) = 0  -  DIAGONAL MODIFICATION NOT CONSIDERED
C               = 1  -  DIAGONAL MODIFICATION CORRESPONDING
C                       TO THE DROPPED FILL-INS IS PERFORMED
C     OPTION(6)      -  NOT USED HERE
C
C IP(I,1),IP(I,2) POINT TO THE START OF ROW/COLUMN I.
C IK(I,1),IK(I,2) HOLD THE NUMBER OF NONZEROES IN ROW/COLUMN I
C     OF THE LOWER TRIANGULAR PART OF A.
C DURING THE MAIN BODY OF THIS SUBROUTINE THE VECTORS
C    IK(*,3),IW(*,1) AND IW(*,2) ARE USED TO HOLD DOUBLY
C    LINKED LISTS OF ROWS THAT HAVE NOT BEEN PIVOTAL AND
C    HAVE EQUAL NUMBER OF NONZEROES.
C IK(I,3) HOLD FIRST ROW/COLUMN TO HAVE I NONZEROS OR
C    ZERO IF THERE ARE NONE.
C IW(I,1) HOLD ROW/COLUMN NUMBER OF ROW/COLUMN PRIOR TO
C    ROW I IN ITS LIST OR ZERO IF NONE.
C IW(I,2) HOLD ROW/COLUMN NUMBER OF ROW/COLUMN AFTER
C     ROW I IN ITS LIST OR ZERO IF NONE.
C DURING THE MAIN BODY OF THE SUBROUTINE INI AND INJ
C   KEEP A COLUMN FILE AND A ROW FILE CONTAINING
C   RESPECTIVELY THE ROW NUMBERS OF THE NONZEROS OF
C   EACH COLUMN AND THE COLUMN NUMBERS OF THE NONZEROS
C   OF EACH ROW.  THE IP ARRAYS POINT TO THE START
C   POSITION IN INI AND INJ OF EACH COLUMN AND ROW.
C
      DATA ZERO,ONE,CMAX/0.0,1.0,1.0E20/
C
C INITIALIZE IK(*,3) AND LOCAL VARIABLES.
      CHANGE=.TRUE.
      IF (C.LE.ZERO) CHANGE=.FALSE.
      NZO=NZ
      IPD=N
      ALFA=1.0/0.90
      B1=-.03
```

```
            B2= .03
            NFILL=IAJ-NZO-N
 65         MCL=LCOL
            CO=0
            IF (OPTION(3).NE.0) CO=ABS(C)/FLOAT(N)
            C=C**2
            DO 5  I=1,N
 70         D(I)=(1+CO)*D(I)
          5 IK(I,3)=0
      C
      C SET UP LINKED LISTS OF ROWS/COLUMNS WITH EQUAL NUMBER
      C   OF NON-ZEROS.
 75   C
            IF (OPTION(1).NE.0) GO TO 9
            DO 8 I=1,N
            IW(I,1)=I-1
            IW(I,2)=I+1
 80     8   CONTINUE
            IW(N,2)=0
            IK(1,3)=1
            GO TO 15
      C
 85     9   CONTINUE
            DO 10 I=1,N
            NZI=IK(I,1)+IK(I,2)+1
            IN= IK(NZI,3)
            IK(NZI,3)=I
 90         IW(I,2)=IN
            IW(I,1)=0
         10 IF (IN.NE.0) IW(IN,1)=I
       15   CONTINUE
      C
 95   C START THE ELIMINATION LOOP
            DO 180 IIP=1,N
      C
      C SEARCH ROWS WITH NRJP NONZEROS.
            DO 20  NRJP=1,N
100         JP=IK(NRJP,3)
            IF(JP.GT.0) GO TO 25
         20 CONTINUE
      C
      C ROW JP  IS USED AS PIVOT.
105   C
      C REMOVE ROWS/COLUMNS INVOLVED IN ELIMINATION FROM
      C    ORDERING VECTORS.
      C
         25 DO 45  L=1,2
110         KPP=IP(JP,L)
```

```
            KLL=IK(JP,L)+ KPP-1
            IF (KPP.GT.KLL) GO TO 45
            DO 40  K=KPP,KLL
            IF (L.EQ.2) GO TO 27
115         J=INJ(K)
            GO TO 28
         27 J=INI(K)
         28 IL=IW(J,1)
            IN=IW(J,2)
120         IW(J,2)=-1
            IF (OPTION(1).EQ.0) GO TO 40
            IF (IN.LT.0) GO TO 40
            IF (IL.EQ.0) GO TO 30
            IW(IL,2)=IN
125         GO TO 35
       30   NZ=IK(J,1)+IK(J,2)+1
            IK(NZ,3)=IN
         35 IF (IN.GT.0) IW(IN,1)=IL
         40 CONTINUE
130      45 CONTINUE
      C
      C REMOVE JP     FROM ORDERING VECTORS
            IL=IW(JP,1)
            IN=IW(JP,2)
135         IW(JP,2) =-10
            IF (OPTION(1).NE.0) GO TO 54
            IK(1,3)=JP+1
            GO TO 55
       54   CONTINUE
140         IF (IN.LT.0) GO TO 55
            NZ=IK(JP,1)+IK(JP,2)+1
            IK(NZ,3)=IN
            IF(IN.GT.0) IW(IN,1)=IL
         55 CONTINUE
145   C
      C  STORE  PIVOT.
            IW(JP,1)=-IP
      C COMPRESS ROW FILE IF NECESSARY.
      C
150         IF(LROW+IK(JP,1)+IK(JP,2).GT.IAJ-N ) C=CMAX
            IF (NURL+IK(JP,1)+IK(JP,2) .LT.NUAL) GO TO 60
            CALL MA31D(A,INJ,IAJ,N,IK,IP,.TRUE.)
         60 KP=IP(JP,1)
            KL=IK(JP,1)+KP-1
155         IP(JP,1)=NURL+1
            IF (KP.GT.KL) GO TO 90
      C
      C REMOVE JP FROM COLUMNS CONTAINED IN THE PIVOT ROW.
```

```
            DO 85  K=KP,KL
160         J=INJ(K)
            KPC=IP(J,2)
            NZ=IK(J,2)-1
            IK(J,2)=NZ
            KLC=KPC+NZ
165         IF (KLC.GT.KPC) GO TO 65
            INI(KPC)=0
            GO TO 80
         65 DO 70  KC=KPC,KLC
            IF (JP.EQ.INI(KC)) GO TO 75
170      70 CONTINUE
         75 INI(KC)=INI(KLC)
            INI(KLC)=0
         80 LCOL=LCOL-1
            NURL=NURL+1
175         INJ(NURL)=J
            A(NURL)=A(K)
         85 INJ(K)=0
      C
      C TRANSFORM COLUMN PART OF PIVOT ROW TO THE ROW FILE.
180      90 KP2=IP(JP,2)
            KL2=IK(JP,2)+KP2-1
            IF (KP2.GT.KL2) GO TO 100
            DO 95  K=KP2,KL2
            NURL=NURL+1
185         LCOL=LCOL-1
            I=INI(K)
            KPR=IP(I,1)
            KLR=KPR+IK(I,1)-1
            DO 92 KR=KPR,KLR
190         IF (JP.EQ.INJ(KR)) GO TO 93
         92 CONTINUE
        93  INJ(KR)=INJ(KLR)
            A(NURL)=A(KR)
            A(KR)=A(KLR)
195         INJ(KLR)=0
            IK(I,1)=IK(I,1)-1
            INJ(NURL)=I
         95 INI(K)=0
        100 NZC=IK(JP,1)+IK(JP,2)
200         IK(JP,1)=NZC
            IK(JP,2)=0
      C
      C UNPACK PIVOT ROW AND CONTROL DIAGONAL VALUE.
            KP=IP(JP,1)
205         KL=KP+NZC-1
            CO=EPSTOL*U
```

```
            IF (KP.GT.KL) GO TO 102
            DO 101 K=KP,KL
            AA=A(K)
210         CO=AMAX1(CO,ABS(AA))
            J=INJ(K)
            W(J)=AA
          101 CONTINUE
          102 DJP=D(JP)
215         IF (DJP.GT.CO/U) GO TO 103
            IFLAG=2
            IF (MP.GT.0) WRITE(MP,250) JP
          250 FORMAT(//44H+ WARNING   MODIFICATION OF ZERO OR NEGATIVE,
             146H DIAGONAL ENTRY HAS BEEN PERFORMED IN LOCATION,I7)
220         D(JP)=CO
            IF (CO.EQ.EPSTOL*U) D(JP)=ONE
          103 IF (KP.GT.KL) GO TO 179
        C
        C PERFORM ROW OPERATIONS.
225         DO 170 NC=1,NZC
            KC=IP(JP,1)+NC-1
            IR=INJ(KC)
            AL=A(KC)/D(JP)
        C
230     C COMPRESS ROW FILE IF NECESSARY.
            IF (LROW+IK(IR,1)+IK(JP,1).GT.IAJ-N) C=CMAX
            IF (NURL+IK(IR,1)+IK(JP,1).LT.NUAL) GO TO 105
            CALL MA31D(A,INJ,IAJ,N,IK,IP,.TRUE.)
          105 KR=IP(IR,1)
235         KRL=KR+IK(IR,1)-1
            IF (KR.GT.KRL) GO TO 120
        C
        C SCAN THE OTHER ROW AND CHANGE SIGN IN IW FOR EACH COMMON
        C    COLUMN NUMBER.
240         DO 115 KS=KR,KRL
            J=INJ(KS)
            IF (IW(J,2).NE.-1) GO TO 115
            IW(J,2)=1
            A(KS)=A(KS)-AL*W(J)
245       115 CONTINUE
        C
        C SCAN PIVOT ROW FOR FILLS.
          120 DO 165  KS=KP,KL
            J=INJ(KS)
250     C
        C  ONLY ENTRIES IN THE UPPER TRIANGULAR PART ARE CONSIDERED.
            IF (J.LT.IR) GO TO 165
            IF(IW(J,2).EQ.1) GO TO 165
            AA=-AL*W(J)
```

```
255         IF(IR.NE.J) GO TO 122
            D(IR)=D(IR)+AA
            GO TO 165
      122   IF (OPTION(2).NE.0) GO TO 123
            IF (FILL(IR,J)) GO TO 124
260         IF (OPTION(5).EQ.0) GO TO 165
            D(J)=D(J)+AA
            D(IR)=D(IR)+AA
            GO TO 165
      123   IF (AA*AA.GT.C*ABS(D(IR)*D(J))) GO TO 124
265         IF (OPTION(5).EQ.0) GO TO 165
            D(J)=D(J)+AA
            D(IR)=D(IR)+AA
            GO TO 165
      124   LROW=LROW+1
270         IK(IR,1)=IK(IR,1)+1
      C  IF POSSIBLE PLACE THE NEW ELEMENT NEXT TO THE PRESENT ENTRY.
      C
      C
      C  TRY IF THERE IS ROOM AT THE END OF THE ENTRY.
275         IF (KR.GT.KRL) GO TO 130
            IF (KRL.EQ.IAJ) GO TO 125
            IF (INJ(KRL+1).NE.0) GO TO 125
            KRL=KRL+1
            INJ(KRL)=J
280         A(KRL)=AA
            GO TO 133
      C
      C  TRY IF THERE IS ROOM AHEAD OF PRESENT ENTRY.
      125   IF (KR.NE.NUAL) GO TO 126
285         NUAL=NUAL-1
            GO TO 127
      126   IF (INJ(KR-1).NE.0) GO TO 128
      127   KR=KR-1
            IP(IR,1)=KR
290         INJ(KR)=J
            A(KR)=AA
            GO TO 133
      C
      C  NEW ENTRY HAS TO BE CREATED.
295   128   DO 129 KK=KR,KRL
            NUAL=NUAL-1
            INJ(NUAL)=INJ(KK)
            A(NUAL)=A(KK)
      129   INJ(KK)=0
300   C
      C  ADD THE NEW ELEMENT.
      130   NUAL=NUAL-1
```

```
            INJ(NUAL)=J
            A(NUAL)=AA
305         IP(IR,1)=NUAL
            KR=NUAL
            KRL=KR+IK(IR,1)-1
      C
      C CREATE FILL IN COLUMN FILE.
310     133 NZ=IK(J,2)
            K=IP(J,2)
            KL1=K+NZ-1
            LCOL=LCOL+1
      C
315   C IF POSSIBLE PLACE NEW ELEMENT AT THE END OF PRESENT ENTRY.
            IF (NZ.EQ.0) GO TO 140
            IF (KL1.EQ.IAI) GO TO 137
            IF (INI(KL1+1).NE.0) GO TO 137
            INI(KL1+1)=IR
320         GO TO 160
      C
      C  IF POSSIBLE PLACE ELEMENT AHEAD OF PRESENT ENTRY.
        137 IF (K.NE.NUCL) GO TO 138
            IF (NUCL.EQ.1) GO TO 140
325         NUCL=NUCL-1
            GO TO 139
        138 IF (INI(K-1).NE.0) GO TO 140
        139 K=K-1
            INI(K)=IR
330         IP(J,2)=K
            GO TO 160
      C
      C NEW ENTRY HAS TO BE CREATED.
        140 IF (NZ+1.LT.NUCL) GO TO 145
335   C
      C COMPRESS COLUMN FILE IF THERE IS NOT ROOM FOR NEW ENTRY.
            IF (LCOL+NZ+2.GE.IAI) C=CMAX
            CALL MA31D(A,INI,IAI,N,IK(1,2),IP(1,2),.FALSE.)
            K=IP(J,2)
340         KL1=K+NZ-1
      C
      C TRANSFER OLD ENTRY INTO NEW.
        145 IF (K.GT.KL1) GO TO 155
            DO 150 KK=K,KL1
345         NUCL=NUCL-1
            INI(NUCL)=INI(KK)
        150 INI(KK)=0
      C
      C ADD THE NEW ELEMENT.
350     155 NUCL=NUCL-1
```

```
            INI(NUCL)=IR
            IP(J,2)=NUCL
          160 IK(J,2)=NZ+1
          165 IW(J,2)=-1
355       170 CONTINUE
      C
      C UPDATE ORDERING ARRAYS.
            DO 172 K=KP,KL
            J=INJ(K)
360         W(J)=0.
            A(K)=A(K)/D(JP)
            IF (OPTION(1).EQ.0) GO TO 171
            NZ=IK(J,1)+IK(J,2)+1
            IN=IK(NZ,3)
365         IW(J,2)=IN
            IW(J,1)=0
            IK(NZ,3)=J
            IF (IN.NE.0) IW(IN,1)=J
            GO TO 172
370       171  IW(J,2)=J+1
            IW(J,1)=J-1
          172  CONTINUE
            IF (OPTION(1).EQ.0) IW(N,2)=0
            MCL=MAX0(MCL,LCOL)
375         PIVT=FLOAT(IIP)/FLOAT(N)
      C
      C  GIVE WARNING IF AVAILABLE SPACE IS USED TOO EARLY.
            IF (C.NE.CMAX) GO TO 175
            IF (IPD.LT.IIP) GO TO 179
380         IPD=IIP
            IF (PIVT .GT. .9) GO TO 179
            IFLAG=4
            IF (MP.GT.0) WRITE(MP,260) IIP
            GO TO 179
385       260 FORMAT(//44H+WARNING  AVAILABLE SPACE USED AT PIVOT STEP,I7)
      C
      C  CHANGE C IF NECESSARY.
          175 IF (.NOT. CHANGE) GO TO 179
            PFILL=FLOAT(LROW-NZ0)/FLOAT(NFILL)
390         IF (PIVT.GT.0.9) GO TO 179
            IF (PFILL.LT.ALFA*PIVT+B1) GO TO 176
            IF (PFILL.LT.ALFA*PIVT+B2) GO TO 179
            C=2.25*C
          176 ALFA=(1.0-PFILL)/(0.9-PIVT)
395         B1=PFILL-PIVT*ALFA-0.03
            B2=B1+0.06
      C
      C  IF THE MATRIX IS FULL  THEN STOP THE SPARSE ANALYZE.
```

```
      179 NR=N-IIP
400       LFULL=NR*(NR-1)/2
          LFULDD=IFIX(DD*FLOAT(LFULL))
          IF (LCOL.GE.LFULDD.AND.NURL+LFULL.LT.IAJ) GO TO 185
      180 CONTINUE
      C
405   C
      C  ELIMINATION LOOP TERMINATES
      C  AFTER DEVIATION WE FACTORIZE THE REMAINING FULL MATRIX.
      185 IPD=IIP
          C=SQRT(C)
410       LCOL=MCL
          IF (.NOT. CHANGE) C=-C
      C
      C  THE ORDER OF THE FULL MATRIX IS NR.
      C  LOOP THROUGH ROWS IN THE ACTIVE MATRIX AND STORE
415   C  ROW NUMBERS IN INI.
          KK=0
          DO 197 I=1,NR
          JP=IK(I,3)
      194 IF (JP)196,196,195
420   195 KK=KK+1
          INI(KK)=JP
          JP=IW(JP,2)
          GO TO 194
      196 IF (KK.EQ.NR) GO TO 198
425   197 CONTINUE
      C
      C  MAKE A SORT OF ROWNUMBERS IN INI.
      198 IF (NR.EQ.1) GO TO 200
          NRM1=NR-1
430       DO 199 I=1,NRM1
          J1=I+1
          DO 199 J=J1,NR
          IF (INI(J).GT.INI(I)) GO TO 199
          JJ=INI(I)
435       INI(I)=INI(J)
          INI(J)=JJ
      199 CONTINUE
      200 DO 201 I=1,NR
          II=INI(I)
440   201 IW(II,1)=-(IPD+I)
      C
      C  MAKE AN ORDERED LIST OF THE PIVOTS.
          DO 202 I=1,N
          IR=-IW(I,1)
445   202 IK(IR,2)=I
      C
```

```
      C  MOVE FULL MATRIX TO THE FRONT AND ORDER.
            IPDP1=IPD+1
            NM1=N-1
450         IF (IPDP1.GT.NM1) GO TO 245
            DO 215 IIP=IPDP1,NM1
            JP=IK(IIP,2)
            KP=IP(JP,1)
            KL=KP+IK(JP,1)-1
455   C
      C   MOVE ROW JP TO W.
            IF (KP.GT.KL) GO TO 204
            DO 203 K=KP,KL
            J=INJ(K)
460         INJ(K)=0
        203 W(J)=A(K)
      C
      C  COMPRESS FILE IF NECESSARY.
        204   IF(NURL+N-IIP.LT.NUAL) GO TO 205
465         CALL MA31D(A,INJ,IAJ,N,IK,IP,.TRUE.)
        205 IP(JP,1)=NURL+1
            IK(JP,1)=N-IIP
      C
      C  MOVE ROWS AND COLUMN INDICES INTO PIVOTAL ORDER.
470         IIPP1=IIP+1
            DO 210 I=IIPP1,N
            J=IK(I,2)
            NURL=NURL+1
            A(NURL)=W(J)
475         INJ(NURL)=J
        210 W(J)=ZERO
        215 CONTINUE
            LROW=NURL
      C
480   C  FACTORIZE THE FULL MATRIX.
            DO 240 IIP=IPDP1,NM1
            JP=IK(IIP,2)
            KPI=IP(JP,1)
            IP1=IIP+1
485         IF (IP1.EQ.N) GO TO 235
      C
      C  LOOP THROUGH THE OTHER ROW
            DO 230 J=IP1,NM1
            JJ=IK(J,2)
490         KPJ=IP(JJ,1)
            KLJ=KPJ+IK(JJ,1)-1
            AL=A(KPI)/D(JP)
            D(JJ)=D(JJ)-AL*A(KPI)
            KK=KPI+1
```

```
495         DO 220 K=KPJ,KLJ
            A(K)=A(K)-AL*A(KK)
      220   KK=KK+1
      C
      C  STORE FACTOR AND PROCEED TO NEXT ROW.
500         A(KPI)=AL
            KPI=KPI+1
      230   CONTINUE
      C
      C  MODIFY LAST DIAGONAL ENTRY
505   235   JJ=IK(N,2)
            AL=A(KPI)/D(JP)
            D(JJ)=D(JJ)-AL*A(KPI)
            A(KPI)=AL
      240   CONTINUE
510   245   CONTINUE
            RETURN
            END
```

```
            LOGICAL FUNCTION FILL(I,J)
      C
      C  FILL1
      C  -----
  5   C
      C  USED WHEN NO FILL-INS ARE TO BE KEPT
      C
            FILL=.FALSE.
            RETURN
 10         END
```

```
            LOGICAL FUNCTION FILL(I,J)
      C
      C  FILL2
      C  -----
  5   C
      C  ALLOWS ONE DIAGONAL OF FILL-INS TO BE KEPT
      C  ADJACENT TO THE OUTER DIAGONAL.
      C
            FILL=.FALSE.
 10         IF (IABS(J-I).GE.7) FILL=.TRUE.
            RETURN
            END
```

```
      LOGICAL FUNCTION FILL(I,J)
C
C  FILL3
C  -----
C
C  ALLOWS THREE DIAGONAL OF FILL-INS TO BE KEPT.
C  ONE ADJACENT TO THE INNER DIAGONAL AND TWO
C  ADJACENT TO THE OUTER DIAGONAL.
C
      FILL=.FALSE.
      ID=IABS(J-I)
      IF ((ID.LE.2).OR.(ID.GE.6)) FILL=.TRUE.
      RETURN
      END



      SUBROUTINE SOLVE(NN,NZ,A,INI,INJ,IAI,IAJ,W,IK,B,W1)
C
C  SUBROUTINE WHICH SOLVES THE LINEAR SYSTEM USING
C  HARWELL'S PRECONDITIONED CONJUGATE GRADIENT
C  ROUTINE MA31F.
C
C  INPUT PARAMETERS
C  ----------------
C
C   NN - ORDER OF MATRIX A.
C   NZ - NUMBER OF NON-ZERO ELEMENTS IN THE UPPER
C        TRIANGULAT PORTION OF MATRIX A.
C   A - ARRAY OF LENGTH IAJ CONTAINING THE NON-ZERO
C       OFF-DIAGONAL ELEMENTS OF THE UPPER TRIANGULAR
C       PORTION OF MATRIX A IN THE FIRST NZ LOCATIONS
C       IN ROW ORDER.  LOCATIONS NZ+1,...,NZ+LROW
C       CONTAIN THE NON-ZERO OFF-DIAGONAL ELEMENTS
C       OF THE UPPER TRIANGULAR PORTION OF THE
C       PRECONDITIONING MATRIX C IN ROW ORDER.
C   INJ - ARRAY OF LENGTH IAJ CONTAINING THE COLUMN
C         INDICES OF THE CORRESPONDING ENTRY IN ARRAY A.
C         (IE. INJ(K) CONTAINS THE COLUMN INDICE FOR
C         ENTRY A(K), K=1,...,NZ+LROW).
C   INI - ARRAY OF LENGTH NZ CONTAINING THE ROW INDICES
C         OF THE CORRESPONDING ENTRY IN ARRAY A.
C         (IE. INI(K) CONTAINS THE ROW INDICE FOR
C         ENTRY A(K), K=1,...,NZ).
C   IAJ - SIZE OF ARRAYS INJ AND A.
C    B - CONTAINS THE RIGHTHAND SIDE OF THE SYSTEM.
C    W - ARRAY OF LENGTH 3*NN IN WHICH LOCATIONS
```

```
      C         1,...,NN CONTAIN THE DIAGONAL ELEMENTS OF
      C         MATRIX A AND LOCATIONS NN+1,...,2*NN CONTAIN
      C         THE INVERSE OF THE DIAGONAL ELEMENTS OF MATRIX C.
      C         THE REMAINING NN LOCATIONS ARE WORK SPACE.
   35 C     W1 - ARRAY OF LENGTH 3*NN USED AS WORK SPACE.
      C
      C  OUTPUT PARAMETERS
      C  -----------------
      C
   40 C     B - THE SOLUTION VECTOR
      C
      C  COMMON BLOCK PARAMETERS
      C  ----------------------
      C
   45 C  LCOL,NCP,IPD,DD - NOT USED
      C  LROW - NUMBER OF NON-ZERO ELEMENTS IN UPPER
      C         TRIANGULAR PORTION OF THE PRECONDITIONING
      C         MATRIX C.
      C  ND - ORDER OF MATRIX A AND C.
   50 C  LP - OUTPUT FILE DEVICE NUMBER.
      C  MP - MESSAGE FILE DEVICE NUMBER.
      C  MITS - MAXIMUM NUMBER OF ITERATIONS TO BE ATTEMPTED.
      C  EPS1 - DESIRED ACCURACY OF !!R!!
      C
   55 C  INTERNAL VARIABLES
      C  ------------------
      C
      C   NITER - ON ENTRY TO MA31F IT CONTAINS THE MAXIMUM
      C           NUMBER OF ITERATION TO BE ATTEMPTED.  ON
   60 C           RETURN FROM MA31F IT CONTAINS THE NUMBER
      C           OF ITERATIONS PERFORMED.
      C    EPS - ON ENTRY TO MA31F, EPS(1) CONTAINS THE
      C          DESIRED ACCURACY FOR !!R!!.  ON RETURN,
      C          EPS(I) CONTAINS THE VALUE OF !!R!! AFTER
   65 C          ITERATION I-1.
      C
            REAL A(IAJ),W(NN,3),W1(NN,3),EPS(150),B(NN)
            INTEGER INI(IAI),INJ(IAJ),IK(NN,2)
      C
   70       COMMON/MA31N/MITS,EPS1
            COMMON/MA31I/DD,LP,MP
            COMMON/MA31J/LROW,LCOL,NCP,ND,IPD
      C
            WRITE(MP,5)
   75    5  FORMAT(12H START SOLVE)
            IAJ1=IAJ-NZ
            NZ1=NZ+1
      C
```

```
      WRITE(LP,292)
 80    292  FORMAT(37HORESULTS OF PRECONDITIONED CG ROUTINE)
      IFLAG=0
      NITER=MITS
      EPS(1)=EPS1
C
 85    CALL SECOND(STRTIM)
C
      CALL MA31F(ND,NZ,A,W,INI,INJ,IAJ1,A(NZ1),W(1,2),
     1INJ(NZ1),IK,B,W(1,3),W1,W1(1,2),W1(1,3),
     2NITER,EPS)
 90  C
      CALL SECOND(STPTIM)
C
      NITER1=NITER+1
      IF (EPS(NITER1).LE.EPS1) GO TO 300
 95    WRITE(LP,295) NITER
  295  FORMAT(20H0--WARNING MORE THAN,I7,2X,
     *47HITERATIONS REQUIRED TO OBTAIN DESIRED ACCURACY.)
      IFLAG=3
C
100   300  WRITE(LP,301) IFLAG
  301  FORMAT(20H0AFTER MA31F IFLAG = ,I2)
      WRITE(LP,305) NITER,EPS(NITER1)
  305  FORMAT(18HONUM ITERATIONS = ,I3,2X,
     *19HNORM OF RESIDUAL = ,E13.5)
105   RTIME=STPTIM-STRTIM
      WRITE(LP,310) RTIME
  310  FORMAT(12HORUN TIME = ,F7.3,4H SEC)
      WRITE(LP,330)
  330  FORMAT(38HONORM OF RESIDUAL AFTER EACH ITERATION)
110   DO 340 I=1,NITER1
      WRITE(LP,335) (I-1),EPS(I)
  335  FORMAT(1H ,I3,2X,E13.5)
  340  CONTINUE
C
115   500  CONTINUE
      RETURN
      END
```

```
      SUBROUTINE MA31F(N,NZ,A,D,INI,INJ,IAF,AF,DF,INJF,IK,B,R,
     1  E,F,G,KMAX,EPS)
C
C  MA31F IS PART OF THE HARWELL MA31 PACKAGE.
C  IT HAS BEEN MODIFIED TO:
C     1)  HANDLE ADDED PARAMETER TO MA31H CALLING SEQUENCE
C     2)  SAVE THE RESULTING RESIDUAL EACH ITERATION
C     3)  USE A RANDOM STARTING VECTOR.
C  SEE ROUTINE MA31A FOR DETAILS.
C
      REAL AF(IAF),DF(N),A(NZ),B(N),R(N),E(N),F(N),G(N),L,D(N)
      REAL EPS(KMAX)
      INTEGER INJF(IAF),INI(NZ),INJ(NZ),IK(N,2)
      DATA  ZERO/0.0/
C
C  THIS SUBROUTINE PERFORMS THE ITERATIVE PROCEDURE.
C  THE PRECONDITIONED CONJUGATE GRADIENT METHOD IS USED.
      DO=ZERO
      EPS1=EPS(1)**2
C
C  COMPUTE THE INITIAL SOLUTION.
      DO 10 I=1,N
   10 E(I)=RANF(I)*2.0
      CALL  MA31G(N,AF,INJF,IAF,DF,IK,E)
C
C  COMPUTE THE RESIDUALS AND INSERT THE INITIAL SOLUTION IN B.
      CALL MA31H(A,D,INI,INJ,NZ,N,E,R)
      R1=ZERO
      DO 20 I=1,N
      R(I)=R(I)-B(I)
      R1=R1+R(I)**2
      G(I)=R(I)
   20 B(I)=E(I)
      KITR=0
      EPS(1)=SQRT(R1)
      IF (R1.LT.EPS1) GO TO 75
C
C  INITIALIZE E AND G.
      CALL MA31G(N,AF,INJF,IAF,DF,IK,G)
      DO 30 I=1,N
      E(I)=-G(I)
   30 DO=DO+R(I)*G(I)
C
C  START ITERATION LOOP
   35 KITR=KITR+1
      CALL MA31H(A,D,INI,INJ,NZ,N,E,F)
      L=ZERO
      DO 40 I=1,N
```

```
      40  L=L+E(I)*F(I)
50        L=DO/L
    C
    C  AJUST B,G AND R.
          R1=ZERO
          DO 50 I=1,N
55        B(I)=B(I)+L*E(I)
          R(I)=R(I)+L*F(I)
          R1=R1+R(I)*R(I)
      50  G(I)=R(I)
          EPS(KITR+1)=SQRT(R1)
60  C
    C  CONTROL THE RESIDUAL.
          IF (R1.LE.EPS1 .OR. KITR.GE.(KMAX-1)) GO TO 75
    C
    C  PROCEED ITERATION .
65        CALL MA31G(N,AP,INJF,IAF,DF,IK,G)
          D1=ZERO
          DO 60 I=1,N
      60  D1=R(I)*G(I)+D1
          BB=D1/DO
70        DO=D1
          DO 70 I=1,N
      70 E(I)=-G(I)+BB*E(I)
          GO TO 35
    C
75  C  ITERATION LOOP TERMINATES.
      75  KMAX=KITR
          RETURN
          END



          SUBROUTINE MA31H(A,D,INI,INJ,NZ,N,B,Z)
    C
    C  MA31H IS PART OF THE HARWELL MA31 PACKAGE.
    C
 5        REAL A(NZ),D(N),B(N),Z(N)
          INTEGER INI(NZ),INJ(NZ)
    C
    C  THIS SUBROUTINE CALCULATES THE INNER PRODUCT OF A MATRIX
    C  A AND A VECTOR B AND THE RESULT IS RETURNED IN VECTOR Z.
10  C  THE DIAGONAL ENTRIES OF MATRIX A ARE CONTAINED IN D.
    C
    C  INITIALIZE A.
    C
          DO 10 I=1,N
```

```
      DO 10 I=1,N
   10 Z(I)=B(I)*D(I)
C
C  LOOP OVER THE NON-ZEROES IN A.
C
      IF (NZ.LE.0) GO TO 100
      DO 90 K=1,NZ
      I=INI(K)
      J=INJ(K)
      Z(I)=Z(I)+A(K)*B(J)
   90 Z(J)=Z(J)+A(K)*B(I)
  100 RETURN
      END



      PROGRAM PROG2(INPUT,OUTPUT,DATA,TAPE4=INPUT,TAPE6=DATA,
     *TAPE5=OUTPUT)
C
C  PROGRAM TO CALCULATE THE EIGENVALUES OF OUR
C  SYMMETRICALLY PRECONDITIONED COEFFICENT MATRIX
C  USING THE HARWELL EA14A LANCZOS ALGORITHM.
C
C  SUBROUTINE GENA AND FACTOR
C  --------------------------
C    SEE PROG1 FOR DESCRIPTION
C
C  SUBROUTINE GETEIG
C  -----------------
C    SUBROUTINE WHICH CALLS SUBROUTINE EA14A TO CALCULATE
C    THE DESIRED EIGENVALUES.
C        MITE - MAXIMUM NUMBER OF ITERATIONS TO BE ATTEMPTED
C        ACC - DESIRED ACCURACY OF RESULTING EIGENVALUES
C        EL,ER - SEARCH INTERVAL
C
C  SEE INDIVIDUAL SUBROUTINES FOR MORE DETAILS.
C
      REAL A(650),B(64),W(64,3)
      INTEGER INI(200),INJ(650),IK(64,4),IW(64,4),OPTION(6)
C
      COMMON/MA31I/DD,LP,MP
      COMMON/MA31J/LROW,LCOL,NCP,ND,IPD
      COMMON/MA31K/NURL,NUCL,NUAL
      COMMON/MCOMM3/OPTION
      COMMON/MA31N/MITE,ACC,EL,ER
      COMMON/MA31L/EPSTOL,U
      COMMON/MA31M/NI,NJ,NVERSN,NTYPE
```

```
      C
            EXTERNAL FILL,EUSE
      C
   35       DATA DD,LP,MP/1.0,6,5/
            DATA EPSTOL,U/2.0E-6,1.0E2/
            DATA IAI,IAJ,NN/200,650,64/
            DATA MITE,ACC,EL,ER/600,1.0E-4,1.0,0.0/
            DATA NI,NJ/8,8/
   40    C
            ND=NN
      C
      C  GET PARAMETERS DETAILING TYPE OF
      C  PRECONDITIONING METHOD TO USE.
   45    C
            READ(4,*) NTYPE,NVERSN
            READ(4,*) (OPTION(I),I=1,6)
            READ(4,*) C
      C
   50       CALL GENA(NN,NZ,A,INI,INJ,IAI,IAJ,W,B,IK,IW)
      C
            IF (OPTION(6).EQ.1) GO TO 5
      C
      C  PERFORM THE DESIRED FACTORIZATION
   55    C
            CALL FACTOR(NN,NZ,A,INI,INJ,IAI,IAJ,IK,IW,W,C,FILL,EUSE)
            GO TO 15
       5    CONTINUE
      C
   60    C  NO PRECONDITIONING REQUESTED
      C  GENERATE IDENTITY MATRIX
      C
            LROW=0
            DO 10 I=1,NN
   65       IK(I,1)=0
            IK(I,2)=I
            W(I,2)=1.0
      10    CONTINUE
      15    CONTINUE
   70    C
      C  CALCULATE THE EIGENVALUES OF THE PRECONDITIONED MATRIX
      C
            CALL GETEIG(NN,NZ,A,INI,INJ,IAI,IAJ,W,IK,B)
      C
   75       END
```

```
      SUBROUTINE GETEIG(NN,NZ,A,INI,INJ,IAI,IAJ,W,IK)
C
C  SUBROUTINE TO CALCULATE ALL THE EIGENVALUES OF
C  OUR SYMMETRICALLY PRECONDITIONED INPUT MATRIX
C  USING THE HARWELL EA14A LANCZOS ALGORITHM.
C  SEE SUBROUTINE SOLVE FOR DESCRIPTION OF INPUT PARAMETERS.
C
      REAL A(IAJ),W(NN,3)
      REAL EIG(1024),U(1024),V(1024),T1(1024),T2(1024)
      REAL X(3000),DEL(3000),ALFA(5000),BETA(5000)
      INTEGER INI(IAI),INJ(IAJ),IK(NN,4)
      INTEGER NU(3000)
C
      COMMON/EA14BD/PRVT(4),IPRVT(6)
      COMMON/MA31I/DD,LP,MP
      COMMON/MA31J/LROW,LCOL,NCP,ND,IPD
      COMMON/MA31N/MITE,ACC,EL,ER
C
      DATA LEIG,LX,LALFA/1024,3000,5000/
C
      NZ1=NZ+1
      IAJ1=IAJ-NZ
      IFLAG=-1
C
C  A MAXIMUM OF MITE ITERATIONS ARE ATTEMPTED TO
C  ACQUIRE ALL EIGENVALUES IN THE INTERVAL EL TO ER
C  TO AN ACCURACY OF ACC.
C
      DO 30 ITER=1,MITE
C
      CALL EA14AD(NN,EL,ER,ACC,LEIG,LX,LALFA,LP,IFLAG,
     *U,V,EIG,NEIG,X,DEL,NU,ALFA,BETA)
C
      IF (IFLAG.EQ.0) GO TO 200
      IF (IFLAG.GT.1) GO TO 100
C
C  CALCULATES VECTOR U = VECTOR U + MATRIX A' TIMES VECTOR V,
C  WHERE MATRIX A' IS THE RESULT OF SYMMETRICALLY
C  PRECONDITIONING MATRIX A BY MATRIX C.
C
      CALL MA31G2(NN,A(NZ1),INJ(NZ1),IAJ1,W(1,2),IK,V,T1)
      CALL MA31H(A,W,INI,INJ,NZ,NN,T1,T2)
      CALL MA31G1(NN,A(NZ1),INJ(NZ1),IAJ1,W(1,2),IK,T2)
C
      DO 20 I=1,NN
      U(I)=U(I) + T2(I)
   20 CONTINUE
C
```

```
      30   CONTINUE
50         GO TO 180
     C
     C  EA14AD IS SIGNALING FAILURE
     C
      100  WRITE(LP,110) IFLAG
55         WRITE(MP,110) IFLAG
      110  FORMAT(26H0EA14AD HAS FAILED. IFLAG=,I2)
           GO TO 290
     C
     C  EA14A COULDN'T FINISH IN THE REQUESTED
60   C  NUMBER OF ITERATIONS.
     C
      180  WRITE(LP,185) MITE
           WRITE(MP,185) MITE
      185  FORMAT(39H0--WARNING ALL EIGENVALUES NOT FOUND IN,
65        *I3,2X,10HITERATIONS)
           ITER=MITE
     C
     C  OUTPUT DATA ON THE CALCULATED EIGENVALUES
     C
70    200  CONTINUE
           WRITE(LP,205) PRVT(1)
      205  FORMAT(19H0SPECTRAL RADIUS = ,E14.7)
           WRITE(LP,215)
      215  FORMAT(30H0DATA ON RESULTING EIGENVALUES)
75         WRITE(LP,220) ITER,ACC
      220  FORMAT(8H ITER = ,I3,2X,6HACC = ,E13.5)
           WRITE(LP,230) NEIG
      230  FORMAT(28H NUM DISTINCT EIGENVALUES = ,I3)
     C
80         DO 235 I=1,NEIG
      235  EIG(I)=EIG(I)-1.0
     C
           WRITE(LP,240)
      240  FORMAT(25H0STATISTICS ON EIG(I)-1.0)
85   C
           CALL DSCRPT(NEIG,1,0,EIG,XMN,STDV,VAR,SKW,XKT,
          *0,0,0,5,LP)
           CALL DSCRP2(NEIG,1,1,0,0,EIG,EIG,XMED,XMIN,XMAX,
          *RNGE,LP)
90   C
      290  CONTINUE
           RETURN
           END
```

```
      SUBROUTINE MA31G1(N,A,INJ,IAJ,D,IK,B)
C
C  SUBROUTINE TO SOLVE A SYSTEM OF EQUATIONS
C    (L TRANSPOSE) (SQRT D) T = B
C  BY BACKWARD SUBSTITUTION.  RESULT IS RETURNED
C  IN VECTOR B.  BASED ON HARWELL ROUTINE MA31G.
C  REMINDER, ARRAY A CONTAINS L TRANSPOSE.
C  SEE MA31G FOR DESCRIPTION OF VARIABLES.
C
      INTEGER INJ(IAJ),IK(N,2)
      REAL A(IAJ),D(N),B(N)
C
      KP=1
C
      DO 25 IIP=1,N
      IC=IK(IIP,2)
      KL=KP+IK(IC,1)-1
      BIC=B(IC)
      IF (KP.GT.KL) GO TO 20
      DO 15 K=KP,KL
      IR=INJ(K)
   15 B(IR)=B(IR)-A(K)*BIC
   20 KP=KL+1
   25 CONTINUE
C
      DO 30 I=1,N
      B(I)=B(I)/SQRT(D(I))
   30 CONTINUE
C
      RETURN
      END



      SUBROUTINE MA31G2(N,A,INJ,IAJ,D,IK,B,T)
C
C  SUBROUTINE TO SOLVE A SYSTEM OF EQUATIONS
C    (SQRT D)(L) T = B
C  BY FORWARD SUBSTITUTION.  BASED ON THE HARWELL
C  ROUTINE MA31G.  SEE MA31G FOR DESCRIPTION OF
C  VARIABLES.
C  REMINDER, ARRAY A CONTAINS L TRANSPOSE.
C
      INTEGER INJ(IAJ),IK(N,2)
      REAL A(IAJ),D(N),B(N),T(N)
      COMMON/MA31J/LROW,LCOL,NCP,ND,IPD
C
```

```
      KL=LROW
15    C
      DO 10 I=1,N
   10 T(I)=B(I)/SQRT(D(I))
      C
      DO 30 IPI=1,N
20    IIP=N+1-IPI
      IR=IK(IIP,2)
      BIR=0.0
      KP=KL-IK(IR,1)+1
      IF (KP.GT.KL) GO TO 25
25    DO 20 K=KP,KL
      IC=INJ(K)
   20 BIR=BIR-A(K)*T(IC)
   25 T(IR)=T(IR)+BIR
      KL=KP-1
30    30 CONTINUE
      C
      RETURN
      END
```

```
      PROGRAM PROG1A(OUTPUT,DATA,TAPE5=OUTPUT,TAPE6=DATA)
C
C  DRIVER PROGRAM USED DURING PHASE III.
C  DESIGNED TO SOLVE THE TEST PROBLEMS USING:
C    A) POINT RED/BLACK GRID POINT ORDERING SCHEME
C      (NTYPE=2)
C    B) INCOMPLETE CHOLESKY FACTORIZATION W/ 0 DIAGONALS
C      ADDED AS PERFORMED BY SUBROUTINE ICCG0.
C  THE FOLLOWING PROGRAM CHANGES ARE REQUIRED BY THE
C   VARIOUS TEST PROBLEMS:
C     1)  TEST PROBLEM 1  (GENA1)
C          NVERSN = 1     NI = 32    NJ = 32
C          ND = 1024
C          USE DIMENSIONS
C               B(1024), W(1024,3), W1(1024,3), IK(1024,2)
C               AND IW(1024)
C     2)  TEST PROBLEM 2  (GENA2)
C          NVERSN = 2     NI = 32    NJ = 31
C          ND = 992
C          USE DIMENSIONS
C               B(992), W(992,3), W1(992,3), IK(992,2)
C               AND IW(992)
C     3)  TEST PROBLEM 3  (GENA3)
C          NVERSN = 3
C          EVERYTHING ELSE AS PER PROBLEM 2
C  SEE PROGRAMS PROG1, GENA, ICCG0 AND SOLVE FOR MORE
C    DETAILS.
C
       REAL A(5000),B(1024),W(1024,3),W1(1024,3)
       INTEGER INI(2000),INJ(5000),IK(1024,2),IW(1024)
C
       COMMON/MA31J/LROW,LCOL,NCP,ND,IPD
       COMMON/MA31N/MITS,EPS1
       COMMON/MA31L/EPSTOL,U
       COMMON/MA31I/DD,LP,MP
       COMMON/MA31M/NI,NJ,NVERSN,NTYPE
C
       DATA U,EPSTOL/1.0E2,2.0E-6/
       DATA MITS,EPS1/100,1.0E-6/
       DATA IAI,IAJ,ND/2000,5000,1024/
       DATA DD,LP,MP/1.0,6,5/
       DATA NI,NJ/32,32/
       DATA NVERSN,NTYPE/1,2/
C
       CALL GENA(ND,NZ,A,INI,INJ,IAI,IAJ,W,B,IK,IW)
       NZ1=NZ+1
       CALL ICCG0(ND,NZ,A,INI,INJ,A(NZ1),INJ(NZ1),IK,
      *IW,W(1,1),W(1,2))
```

```
      IAJ2=NZ+LROW
50    CALL SOLVE(ND,NZ,A,INI,INJ,NZ,IAJ2,W,IK,B,W)
C
      END



      PROGRAM PROG1B(OUTPUT,DATA,TAPE5=OUTPUT,TAPE6=DATA)
C
C  DRIVER PROGRAM USED DURING PHASE III.
C  DESIGNED TO SOLVE THE TEST PROBLEMS USING
 5C    A) LINE RED/BLACK GRID POINT ORDERING SCHEME
C        (NTYPE = 1)
C     B) CHOLESKY FACTORIZATION OF THE BLOCK TRIDIAGONAL
C        PORTION OF MATRIX A, AS PERFORMED BY SUBROUTINE BDIAG.
C  SEE PROG1A FOR PROGRAM SET-UP ASSOCIATED WITH EACH OF
10C  THE TEST PROBLEMS.
C  SEE PROG1, GENA, BDIAG AND SOLVE FOR MORE DETAILS.
C
      REAL A(5000),B(992),W(992,3),W1(992,3)
      INTEGER INI(2000),INJ(5000),IK(992,2),IW(992)
15C
      COMMON/MA31J/LROW,LCOL,NCP,ND,IPD
      COMMON/MA31N/MITS,EPS1
      COMMON/MA31L/EPSTOL,U
      COMMON/MA31I/DD,LP,MP
20    COMMON/MA31M/NI,NJ,NVERSN,NTYPE
C
      DATA U,EPSTOL/1.0E2,2.0E-6/
      DATA MITS,EPS1/150,1.0E-6/
      DATA IAI,IAJ,ND/2000,5000,992/
25    DATA DD,LP,MP/1.0,6,5/
      DATA NI,NJ/32,31/
      DATA NVERSN,NTYPE/2,1/
C
      CALL GENA(ND,NZ,A,INI,INJ,IAI,IAJ,W,B,IK,IW)
30    NZ1=NZ+1
      CALL BDIAG(ND,NZ,A,INI,INJ,A(NZ1),INJ(NZ1),IK,
     *IW,W(1,1),W(1,2))
      IAJ2=NZ+LROW
      CALL SOLVE(ND,NZ,A,INI,INJ,NZ,IAJ2,W,IK,B,W1)
35C
      END
```

```
      PROGRAM PROG1C(OUTPUT,DATA,TAPE5=OUTPUT,TAPE6=DATA)
C
C  DRIVER PROGRAM USED DURING PHASE III.
C  DESIGNED TO SOLVE TEH TEST PROBLEMS USING
C   A)  2 LINE RED/BLACK GRID POINT ORDERING SCHEME
C       (NTYPE = 3)
C   B)  REDUCED BLOCK INCOMPLETE CHOLESKY FACTORIZATION
C       WITH 0 DIAGONALS ADDED AS PERFORMED BY RBIC0.
C  SEE PROG1A FOR PROGRAM SET-UP ASSOCIATED WITH EACH OF
C  THE TEST PROBLEMS.
C  SEE PROG1, GENA, RBIC0 AND SOLVE FOF MORE DETAILS.
C
      REAL A(5000),B(1024),W(1024,3),W1(1024,3)
      INTEGER INI(2000),INJ(5000),IK(1024,2),IW(1024)
C
      COMMON/MA31J/LROW,LCOL,NCP,ND,IPD
      COMMON/MA31N/MITS,EPS1
      COMMON/MA31L/EPSTOL,U
      COMMON/MA31I/DD,LP,MP
      COMMON/MA31M/NI,NJ,NVERSN,NTYPE
C
      DATA U,EPSTOL/1.0E2,2.0E-6/
      DATA MITS,EPS1/100,1.0E-6/
      DATA IAI,IAJ,ND/2000,5000,1024/
      DATA DD,LP,MP/1.0,6,5/
      DATA NI,NJ/32,32/
      DATA NVERSN,NTYPE/1,3/
C
      CALL GENA(NDNZ,A,INI,INJ,IAI,IAJ,W,B,IK,IW)
      NZ1=NZ+1
      NCP=NJ
      CALL RBIC0(ND,NZ,A,INI,INJ,A(NZ1),INJ(NZ1),IK,
     *IW,W(1,1),W(1,2))
      IAJ2=NZ+LROW
      CALL SOLVE(ND,NZ,A,INI,INJ,NZ,IAJ2,W,IK,B,W1)
C
      END
```

```
      PROGRAM PROG1D(OUTPUT,DATA,TAPE5=OUTPUT,TAPE6=DATA)
C
C  DRIVER PROGRAM USED DURING PHASE III.
C  DESIGNED TO SOLVE THE TEST PROBLEMS USING
C   A)  NATURAL GRID POINT ORDERING SCHEME (NTYPE = 0)
C   B)  NO PRECONDITIONING
C  SEE PROG1A FOR PROGRAM SET-UP ASSOCIATED WITH EACH OF
C  THE TEST PROBLEMS.
C  SEE PROG1, GENA AND SOLVE FOR MORE DETAILS.
C
      REAL A(5000),B(1024),W(1024,3),W1(1024,3)
      INTEGER INI(2000),INJ(5000),IK(1024,2),IW(1024)
C
      COMMON/MA31J/LROW,LCOL,NCP,ND,IPD
      COMMON/MA31N/MITS,EPS1
      COMMON/MA31L/EPSTOL,U
      COMMON/MA31I/DD,LP,MP
      COMMON/MA31M/NI,NJ,NVERSN,NTYPE
C
      DATA U,EPSTOL/1.0E2,2.0E-6/
      DATA MITS,EPS1/100,1.0E-6/
      DATA IAI,IAJ,ND/2000,5000,1024/
      DATA DD,LP,MP/1.0,6,5/
      DATA NI,NJ/32,32/
      DATA NVERSN,NTYPE/1,0/
C
      CALL GENA(ND,NZ,A,INI,INJ,IAI,IAJ,W,B,IK,IW)
      LROW=0
      DO 10 I=1,ND
      IK(I,1)=0
      IK(I,2)=I
      W(I,2)=1.0
   10 CONTINUE
C
      WRITE(LP,15)
   15 FORMAT(19H NO PRECONDITIONING)
      IAJ2=NZ+LROW
      CALL SOLVE(ND,NZ,A,INI,INJ,NZ,IAJ2,W,IK,B,W1)
C
      END
```

```
      SUBROUTINE GENA(NN,NZ,A,INI,INJ,IAI,IAJ,D,B,IK,IW)
C
C*************************************************
C
C   GENA2
C   -----
C
C   PERFORMS THE DISCRETIZATION OF MODEL PROBLEM 2.
C   SEE GENA1 FOR DESCRIPTION OF VARIABLES.
C
C*************************************************
C
      REAL A(IAJ),B(NN),D(NN),ATYPE(4)
      INTEGER INI(IAI),INJ(IAJ),IK(NN,2),IW(NN)
C
      COMMON/MA31J/LROW,LCOL,NCP,ND,IPD
      COMMON/MA31I/DD,LP,MP
      COMMON/MA31M/NI,NJ,NVERSN,NTYPE
C
      DATA ATYPE/7HNATURAL,7HLINE RB,8HPOINT RB,8H2LINE RB/
      WRITE(MP,2)
    2 FORMAT(11H GENA START)
C
      DO 5 I=1,ND
      IK(I,1)=0
      IK(I,2)=0
      IW(I)=0
    5 CONTINUE
C
      CALL TIME(AT)
      CALL DATE(AD)
      CALL SECOND(TIM1)
C
      NNAT=0
      NZ=0
C
      DO 100 I=1,NI
      DO 90 J=1,NJ
      NNAT=NNAT+1
      N=NORDER(NTYPE,I,J,NNAT)
      D(N)=4.0
      B(N)=0.0
      IF (I.EQ.1) D(N)=D(N)/2.0
      IF (J.EQ.NJ) D(N)=D(N)/2.0
      IF (I.EQ.NI) D(N)=D(N)/2.0
      IF (J.NE.1) GO TO 10
      B(N)=1.0
      IF ((I.EQ.1).OR.(I.EQ.NI)) B(N)=0.5
```

```
 10   CONTINUE
C
C  CALCULATE INNER DIAGONAL
C
      IF (J.EQ.NJ) GO TO 20
      NZ=NZ+1
      A(NZ)=-1.0
      IF ((I.EQ.1).OR.(I.EQ.NI)) A(NZ)=-0.5
      NT=NORDER(NTYPE,I,J+1,NNAT+1)
      CALL ISTORE(N,NT,INI,INJ,IAI,IK,ND,NZ)
 20   CONTINUE
C
C  CALCULATE OUTER DIAGONAL
C
      IF (I.EQ.NI) GO TO 90
      NZ=NZ+1
      A(NZ)=-1.0
      IF (J.EQ.NJ) A(NZ)=-0.5
      NT=NORDER(NTYPE,I+1,J,NNAT+NJ)
      CALL ISTORE(N,NT,INI,INJ,AI,IK,ND,NZ)
 90   CONTINUE
 100  CONTINUE
C
C  INITIALIZE IW(I) TO POINT JUST BEYOND WHERE THE
C  LAST COMPONENT OF ROW I WILL BE STORED
C
      KI=1
      DO 200 I=1,ND
      KI=KI+IK(I,1)
 200  IW(I)=KI
C
C  REORDER BY ROWS USING IN-PLACE SORT ALGORITHM
C
      CALL MA31E(INI,INJ,NZ,IW,ND,A)
C
C  REINITIALIZE IW(I) TO POINT TO THE BEGINNING OF ROW I
C
      KK=1
      DO 210 IR=1,ND
      IW(IR)=KK
 210  KK=KK+IK(IR,1)
      DO 220 I=1,NZ
 220  INI(I)=IABS(INI(I))
C
      CALL SECOND(TIM2)
      TIMD=TIM2-TIM1
C
      WRITE(LP,250) TIMD
```

```
      250  FORMAT(13H GENA TIME = ,F6.3,4H SEC)
           WRITE(LP,260) NVERSN
      260  FORMAT(11H VERSION = ,I2)
100        WRITE(LP,265) ATYPE(NTYPE+1)
      265  FORMAT(14H MATRIX A HAS ,A10,9H ORDERING)
           WRITE(LP,270) AD,AT
      270  FORMAT(18H DATE GENERATED = ,A10,A10)
           WRITE(LP,280) ND,NZ
105   280  FORMAT(6H ND = ,I4,6H NZ = ,I4)
           WRITE(MP,290)
      290  FORMAT(9H GENA END)
     C
           RETURN
110        END



           SUBROUTINE GENA(NN,NZ,A,INI,INJ,IAI,IAJ,D,B,IK,IW)
     C
     C*****************************************************
     C
  5  C    GENA3
     C    -----
     C
     C    PERFORMS THE DISCRETIZATION OF MODEL PROBLEM 3.
     C    SEE GENA1 FOR DESCRIPTION OF VARIABLES.
 10  C
     C*****************************************************
     C
           REAL A(IAJ),B(NN),D(NN),ATYPE(4)
           INTEGER INI(IAI),INJ(IAJ),IK(NN,2),IW(NN)
 15  C
           COMMON/MA31J/LROW,LCOL,NCP,ND,IPD
           COMMON/ADATA/NT,NV,AD,AT
           COMMON/MA31I/DD,LP,MP
           COMMON/MA31M/NI,NJ,NVERSN,NTYPE
 20  C
           DATA ATYPE/7HNATURAL,7HLINE RB,8HPOINT RB,8H2LINE RB/
           WRITE(MP,2)
      2    FORMAT(11H GENA START)
     C
 25        DO 5 I=1,ND
           IK(I,1)=0
           IK(I,2)=0
           IW(I)=0
      5    CONTINUE
 30  C
```

```
      CALL TIME(AT)
      CALL DATE(AD)
      CALL SECOND(TIM1)
C
35    NNAT=0
      NZ=0
      H=1.0/31.0
      HD2=H/2.0
      H2=2.0*H
40    HSQ=H*H
C
      X=-H
      XP1=-HD2
      XP1SQ=XP1*XP1
45  C
      DO 95 I=1,NI
C
      XS1=XP1
      XS1SQ=XP1SQ
50    XP1=XS1+H
      XP1SQ=XP1*XP1
      X=X+H
      XSQ=X*X
C
55    Y=0.0
      YP1=HD2
      CYP=EXP(X*YP1)
C
      DO 95 J=1,NJ
60  C
      Y=Y+H
      YS1=YP1
      YP1=YS1+H
      YSQ=Y*Y
65  C
      NNAT=NNAT+1
      N=NORDER(NTYPE,I,J,NNAT)
C
      AXS=XS1SQ+YSQ+1.0
70    AXP=XP1SQ+YSQ+1.0
      CYS=CYP
      CYP=EXP(X*YP1)
C
      GXY=4.0*YSQ*(XSQ+YSQ+1.0)+6.0*Y
75    GXY=XSQ*GXY+2.0*Y*(YSQ+1.0)
      GXY=1.0-GXY-XSQ*(XSQ+X)*EXP(X*Y)
      GXY=EXP(XSQ*Y)*GXY
C
```

```
            D(N)=AXS+AXP+CYS+CYP+HSQ
80          B(N)=HSQ*GXY
      C
            IF (I.EQ.1) GO TO 25
            IF (I.EQ.NI) GO TO 50
      C
85          IF (J.EQ.1) GO TO 10
            IF (J.NE.NJ) GO TO 15
      C
            D(N)=(D(N)+H2*CYP)/2.0
            B(N)=(B(N)+H2*CYP*EXP(XSQ)*(1.0+XSQ))/2.0
90          NZ=NZ+1
            A(NZ)=-AXP/2.0
            GO TO 20
      C
       10   B(N)=B(N)+CYS
95     15   NZ=NZ+1
            A(NZ)=-CYP
            NT=NORDER(NTYPE,I,J+1,NNAT+1)
            CALL ISTORE(N,NT,INI,INJ,IAI,IK,ND,NZ)
            NZ=NZ+1
100         A(NZ)=-AXP
       20   NT=NORDE(NTYPE,I+1,J,NNAT+NJ)
            CALL ISTORE(N,NT,INI,INJ,IAI,IK,ND,NZ)
            GO TO 95
      C
105    25   D(N)=D(N)/2.0
            B(N)=B(N)/2.0
            IF (J.NE.1) GO TO 30
            B(N)=B(N)+CYS/2.0
            GO TO 35
110   C
       30   IF (J.NE.NJ) GO TO 35
            T1=H2*CYP/4.0
            D(N)=D(N)/2.0+T1
            B(N)=B(N)/2.0+T1
115         NZ=NZ+1
            A(NZ)=-AXP/4.0
            GO TO 40
      C
       35   NZ=NZ+1
120         A(NZ)=-CYP/2.0
            NT=NORDER(NTYPE,I,J+1,NNAT+1)
            CALL ISTORE(N,NT,INI,INJ,IAI,IK,ND,NZ)
            NZ=NZ+1
            A(NZ)=-AXP/2.0
125    40   NT=NORDER(NTYPE,I+1,J,NNAT+NJ)
            CALL ISTORE(N,NT,INI,INJ,IAI,IK,ND,NZ)
```

```
            GO TO 95
      C
       50   IF (J.EQ.NJ) GO TO 55
130         D(N)=D(N)/2.0
            B(N)=B(N)+4.0*H*Y*EXP(Y)*AXP
            IF (J.EQ.1) B(N)=B(N)+CYS
            B(N)=B(N)/2.0
            NZ=NZ+1
135         A(NZ)=-CYP/2.0
            NT=NORDER(NTYPE,I,J+1,NNAT+1)
            CALL ISTORE(N,NT,INI,INJ,IAI,IK,ND,NZ)
            GO TO 95
      C
140    55   D(N)=(D(N)+H2*CYP)/4.0
            B(N)=B(N)/4.0+H*EXP(1.0)*(AXP+CYP)
      C
       95   CONTINUE
      C
145   C  INITIALIZE IW(I) TO POINT JUST BEYOND WHERE THE
      C  LAST COMPONENT OF ROW I WILL BE STORED
      C
            KI=1
            DO 200 I=1,ND
150         KI=KI+IK(I,1)
       200  IW(I)=KI
      C
      C  REORDER BY ROWS USING IN-PLACE SORT ALGORITHM
      C
155         CALL MA31E(INI,INJ,NZ,IW,ND,A)
      C
      C  REINITIALIZE IW(I) TO POINT TO THE BEGINNING OF ROW I
      C
            KK=1
160         DO 210 IR=1,ND
            IW(IR)=KK
       210  KK=KK+IK(IR,1)
            DO 220 I=1,NZ
       220  INI(I)=IABS(INI(I))
165   C
            CALL SECOND(TIM2)
            TIMD=TIM2-TIM1
      C
            WRITE(LP,250) TIMD
170    250  FORMAT(13H GENA TIME = ,F6.3,4H SEC)
            WRITE(LP,260) NVERSN
       260  FORMAT(11H VERSION = ,I2)
            WRITE(LP,265) ATYPE(NTYPE+1)
       265  FORMAT(14H MATRIX A HAS ,A10,9H ORDERING)
```

```
      WRITE(LP,270) AD,AT
  270 FORMAT(18H DATE GENERATED = ,A10,A10)
      WRITE(LP,280) ND,NZ
  280 FORMAT(6H ND = ,I4,6H NZ = ,I4)
      WRITE(MP,290)
  290 FORMAT(9H GENA END)
C
      RETURN
      END



      SUBROUTINE ICCGO(NN,NZA,A,INI,INJ,C,INJC,IK,IW,DA,DC)
C
C  SUBROUTINE TO CALCULATE THE INCOMPLETE CHOLESY
C  FACTORIZATION WITH ZERO FILL-IN OF THE INPUT
C  MATRIX A.
C
C  INPUT PARAMETERS
C  ----------------
C
C   NN - ORDER OF MATRIX A
C   NZA - NMBER OF NON-ZERO ELEMENTS IN THE UPPER
C         TRIANGULAR PORTION OF MATRIX A
C   A - ARRAY CONTAINING THE NON-ZERO ELEMENTS IN THE
C       UPPER TRIANGULAR PORTION OF MATRIX A IN ROW
C       ORDER
C   INI/INJ - ARRAYS CONTAINING THE ROW/COLUMN INDICES
C             OF THE CORRESPONDING ENTRY IN ARRAY A.
C            (IE. INI(I) AND INJ(I) CONTAIN THE ROW
C             AND COLUMN INDICE FOR ENTRY A(I))
C   IK(I,1) - CONTAINS THE NUMBER OF ELEMENTS IN
C             ARRAY A BELONGING TO ROW I
C   IW(I) - POINTS TO THE START OF ROW I IN ARRAY A
C   DA - ARRAY CONTAINING THE DIAGONAL ELEMENTS OF
C        MATRIX A
C
C  OUTPUT PARAMETERS
C  -----------------
C
C   C - ARRAY CONTAINING THE NON-ZERO ELEMENTS IN THE
C       UPPER TRIANGULAR PORTION OF THE INCOMPLETE
C       CHOLESKY FACTORIZATION
C   INJC - ARRAY CONTAINING THE COLUMN INDEX OF THE
C          CORRESPONDING ENTRY IN ARRAY C
C   DC - ARRAY CONTAINING THE DIAGONAL ELEMENTS IN
C        THE INCOMPLETE CHOLESKY FACTORIZATION
```

```
      C   IK(I,1) - NUMBER OF NON-ZERO ELEMENTS IN ROW I
      C             OF THE INCOMPLETE FACTORIZATION
      C   IK(I,2) - USED BY OTHER HARWELL ROUTINES TO
      C             IDENTIFY THE ORDER IN WHICH THE ROWS
   40 C             WERE PROCESSED.  IN THIS CASE, ROWS
      C             PROCESSED IN NATURAL ORDER AND
      C             IK(I,2) = I
      C
      C  COMMON BLOCK PARAMETERS
   45 C  ----------------------
      C
      C   DD,LCOL,NCP,IPD - NOT USED
      C   LP - OUTPUT FILE UNIT NUMBER
      C   MP - MESSAGE FILE UNIT NUMBER
   50 C   LROW - NUMBER OF NON-ZERO ELEMENTS IN THE UPPER
      C          TRIANGULAR PORTION OF THE INCOMPLETE
      C          FACTORIZATION
      C   ND - ORDER OF MATRIX A
      C   EPSTOL - MINIMUM SIZE FOR DIAGONAL ELEMENT
   55 C   U - PARAMETER USED TO DETERMINE WHEN A DIAGONAL
      C       ELEMENT MUST BE MODIFIED TO INSURE POSITIVE
      C       DEFINITENESS
      C
            INTEGER IK(NN,2),IW(NN),INI(NZA),INJ(NZA),INJC(NZA)
   60       REAL A(NZA),DA(NN),DC(NN),C(NZA)
      C
            COMMON/MA31I/DDLP,MP
            COMMON/MA31J/LROW,LCOL,NCP,ND,IPD
            COMMON/MA31L/EPSTOL,U
   65 C
            CALL SECOND(TIM1)
      C
            WRITE(MP,2)
       2    FORMAT(12H START ICCG0)
   70       WRITE(LP,3)
       3    FORMAT(26H PRECONDITIONING = ICCG(0))
      C
            IDC=0
            CT=EPSTOL*U
   75       IRC=0
      C
            DO 5 K=1,ND
       5    DC(K)=DA(K)
      C
   80       DO 100 IROW=1,ND
            IRS=IW(IROW)
            IRE=IRS+IK(IROW,1)-1
            IK(IROW,1)=0
```

```
      IK(IROW,2)=IROW
C
C  DETERMINE IF DIAGONAL ELEMENT MUST BE MODIFIED
C  TO PRESERVE POSITIVE DEFINITENESS
C
      CO=CT
      IF (IRS.GT.IRE) GO TO 20
      DO 10 K=IRS,IRE
   10 CO=AMAX1(CO,ABS(A(K)))
   20 IF (DC(IROW).GT.(CO/U)) GO TO 30
      IDC=IDC+1
      DC(IROW)=CO
      IF (CO.EQ.CT) DC(IROW)=1.0
   30 CONTINUE
C
C  PROCESS ELEMENTS IN CURRENT ROW
C
      IF (IRS.GT.IRE) GO TO 100
      DO 90 IR=IRS,IRE
      I=INI(IR)
      J=INJ(IR)
      IRC=IRC+1
      T=A(IR)
      C(IRC)=T/DC(IROW)
      INJC(IRC)=J
      DC(J)=DC(J)-T*C(IRC)
      IK(IROW,1)=IK(IROW,1)+1
   90 CONTINUE
C
  100 CONTINUE
C
      LROW=IRC
      CALL SECOND(TIM2)
      TIMD=TIM2-TIM1
C
C   OUTPUT STATISTICS
C
      WRITE(LP,110) TIMD
  110 FORMAT(14H ICCG0 TIME = ,F6.3,5H SECS)
      WRITE(LP,120) LROW
  120 FORMAT(8H LROW = ,I4)
      IF (IDC.NE.0) WRITE(LP,130) IDC
  130 FORMAT(4H ** ,I4,19H DIAGONALS MODIFIED)
      WRITE(MP,140)
  140 FORMAT(10H ICCG0 END)
C
      RETURN
      END
```

```
      SUBROUTINE BDIAG(NN,NZA,A,INI,INJ,C,INJC,IK,IW,DA,DC)
C
C  SUBROUTINE TO CALCULATE THE CHOLESKY FACTORIZATION
C  OF THE TRI-DIAGONAL PORTION OF THE INPUT MATRIX A.
C
C  SEE SUBROUTINE ICCGO FOR DESCRIPTION OF PARAMETERS.
C
      REAL A(NZA),DA(NN),DC(NN),C(NZA)
      INTEGER IK(NN,2),IW(NN),INI(NZA),INJ(NZA),INJC(NZA)
C
      COMMON/MA31I/DD,LP,MP
      COMMON/MA31J/LROW,LCOL,NCP,ND,IPD
      COMMON/MA31L/EPSTOL,U
C
      CALL SECOND(TIM1)
C
      WRITE(MP,2)
    2 FORMAT(12H START BDIAG)
      WRITE(LP,3)
    3 FORMAT(37H PRECONDITIONING = BLOCK TRI-DIAGONAL)
C
      IDC=0
      CT=EPSTOL*U
      IRC=0
C
      DO 5 K=1,ND
    5 DC(K)=DA(K)
C
      DO 100 IROW=1,ND
      IRS=IW(IROW)
      IRE=IRS+IK(IROW,1)-1
      IK(IROW,1)=0
      IK(IROW,2)=IROW
C
C  DETERMINE IF DIAGONAL ELEMENT MUST BE MODIFIED
C  TO PRESERVE POSTIVE DEFINITENESS
C
      CO=CT
      IF (IRS.GT.IRE) GO TO 20
      DO 10 K=IRS,IRE
   10 CO=AMAX1(CO,ABS(A(K)))
   20 IF (DC(IROW).GT.(CO/U)) GO TO 30
      IDC=IDC+1
      DC(IROW)=CO
      IF (CO.EQ.CT) DC(IROW)=1.0
   30 CONTINUE
C
C  PROCESS ELEMENTS IN THE CURRENT ROW
```

```
      C
50          IF (IRS.GT.IRE) GO TO 100
            DO 90 IR=IRS,IRE
            I=INI(IR)
            J=INJ(IR)
            IF ((J-I).GT.1) GO TO 90
55          IRC=IRC+1
            T=A(IR)
            C(IRC)=T/DC(IROW)
            INJC(IRC)=J
            DC(J)=DC(J)-T*C(IRC)
60          IK(IROW,1)=IK(IROW,1)+1
       90   CONTINUE
       100  CONTINUE
      C
            LROW=IRC
65          CALL SECOND(TIM2)
            TIMD=TIM2-TIM1
      C
      C  OUTPUT STATISTICS
      C
70          WRITE(LP,110) TIMD
       110  FORMAT(14H BDIAG TIME = ,F6.3,5H SECS)
            WRITE(LP,120) LROW
       120  FORMAT(8H LROW = ,I4)
            IF (IDC.NE.0) WRITE(LP,130) IDC
75     130  FORMAT(4H ** ,I4,19H DIAGONALS MODIFIED)
            WRITE(MP,140)
       140  FORMAT(10H BDIAG END)
      C
            RETURN
80          END



            SUBROUTINE RBICO(NN,NZA,A,INI,INJ,C,INJC,IK,IW,DA,DC)
      C
      C  SUBROUTINE TO CALCULATE THE INCOMPLETE CHOLESKY
      C  FACTORIZATION OF THE QUINT-DIAGONAL PORTION OF
 5    C  THE INPUT MATRIX A.  IT IS ASSUMED THAT THE
      C  2 LINE RED/BLACK ORDERING OF GRID POINTS WAS
      C  USED IN GENERATING MATRIX A.
      C
      C  SEE SUBROUTINE ICCGO FOR DESCRIPTION OF PARAMETERS
10    C
      C  NCP - DISTANCE FROM MAIN DIAGONAL TO OUTER MOST
      C         DIAGONAL TO BE INCLUDED IN THE INCOMPLETE
```

```
      C        FACTORIZATION.
      C
      REAL A(NZA),DA(NN),DC(NN),C(NZA)
      INTEGER IK(NN,2),IW(NN),INI(NZA),INJ(NZA),INJC(NZA)
      C
      COMMON/MA31I/DD,LP,MP
      COMMON/MA31J/LROW,LCOL,NCP,ND,IPD
      COMMON/MA31L/EPSTOL,U
      C
      CALL SECOND(TIM1)
      C
      WRITE(MP,2)
    2 FORMAT(12H START RBIC0)
      WRITE(LP,3)
    3 FORMAT(26H PRECONDITIONING = RBIC(0))
      C
      IDC=0
      CT=EPSTOL*U
      IRC=0
      C
      DO 5 K=1,ND
    5 DC(K)=DA(K)
      C
      DO 100 IROW=1,ND
      IRS=IW(IROW)
      IRE=IRS+IK(IROW,1)-1
      IK(IROW,1)=0
      IK(IROW,2)=IROW
      C
      C  DETERMINE IF DIAGONAL ELEMENT MUST BE MODIFIED
      C  TO PRESERVE POSITIVE DEFINITENESS
      C
      CO=CT
      IF (IRS.GT.IRE) GO TO 20
      DO 10 K=IRS,IRE
   10 CO=AMAX1(CO,ABS(A(K)))
   20 IF (DC(IROW).GT.(CO/U)) GO TO 30
      IDC=IDC+1
      DC(IROW)=CO
      IF (CO.EQ.CT) DC(IROW)=1.0
   30 CONTINUE
      C
      C  PROCESS ELEMENTS IN CURRENT ROW
      C
      IF (IRS.GT.IRE) GO TO 100
      DO 90 IR=IRS,IRE
      I=INI(IR)
      J=INJ(IR)
```

```
            IF ((J-I).GT.NCP) GO TO 90
            IRC=IRC+1
            T=A(IR)
            C(IRC)=T/DC(IROW)
65          INJC(IRC)=J
            DC(J)=DC(J)-T*C(IRC)
            IK(IROW,1)=IK(IROW,1)+1
       90   CONTINUE
       100  CONTINUE
70     C
            LROW=IRC
            CALL SECOND(TIM2)
            TIMD=TIM2-TIM1
       C
75     C  OUTPUT STATISTICS
       C
            WRITE(LP,110) TIMD
       110  FORMAT(14H RBICO TIME = ,F6.3,5H SECS)
            WRITE(LP,120) LROW
80     120  FORMAT(8H LROW = ,I4)
            IF (IDC.NE.0) WRITE(LP,130) IDC
       130  FORMAT(4H ** ,I4,19H DIAGONALS MODIFIED)
            WRITE(MP,140)
       140  FORMAT(10H RBICO END)
85     C
            RETURN
            END
```

```
      PROGRAM PROG2A(OUTPUT,DATA,TAPE5=OUTPUT,TAPE6=DATA)
C
C  DRIVER PROGRAM USED DURING PHASE III.
C  DESIGNED TO FIND THE EXTREME EIGENVALUES OF THE
C  SYMMETRICALLY PRECONDITIONED TEST MATRICES.
C  IT USES:
C   A)  POINT RED/BLACK GRID POINT ORDERING SCHEME (NTYPE = 2)
C   B)  INCOMPLETE CHOLESKY FACTORIZATION WITH 0 DIAGONALS
C       ADDED, AS PERFORMED BY SUBROUTINE ICCG0.
C  SEE PROG1A FOR PROGRAM SET-UP ASSOCIATED WITH EACH OF
C  THE TEST PROBLEMS.
C  SEE PROG2, GENA, ICCG0 AND GETEG2 FOR MORE DETAILS.
C
      REAL A(5000),B(1024),W(1024,3),W1(1024,3)
      INTEGER INI(2000),INJ(5000),IK(1024,2),IW(1024)
C
      COMMON/MA31J/LROW,LCOL,NCP,ND,IPD
      COMMON/MA31N/MITE,ACC,EL,ER
      COMMON/MA31L/EPSTOL,U
      COMMON/MA31I/DD,LP,MP
      COMMON/MA31M/NI,NJ,NVERSN,NTYPE
C
      DATA U,EPSTOL/1.0E2,2.0E-6/
      DATA MITE,ACC,EL,ER/750,1.0E-2,0.0,1.2/
      DATA IAI,IAJ,ND/2000,5000,1024/
      DATA DD,LP,MP/1.0,6,5/
      DATA NI,NJ/32,32/
      DATA NVERSN,NTYPE/1,2/
C
      CALL GENA(ND,NZ,A,INI,INJ,IAI,IAJ,W,B,IK,IW)
      NZ1=NZ+1
      CALL ICCG0(ND,NZ,A,INI,INJ,A(NZ1),INJ(NZ1),IK,IW,
     *W(1,1),W(1,2))
      IAJ2=NZ+LROW
      CALL GETEG2(ND,NZ,A,INI,INJ,NZ,IAJ2,W,IK)
C
      END
```

```
      PROGRAM PROG2B(OUTPUT,DATA,TAPE5=OUTPUT,TAPE6=DATA)
C
C  DRIVER PROGRAM USED DURING PHASE III.
C  DESIGNED TO FIND THE EXTREME EIGENVALUES OF THE
C  SYMMETRICALLY PRECONDTIONED TEST MATRICES.
C  IT USES:
C   A)  LINE RED/BLACK GRID POINT ORDERING SCHEME (NTYPE = 1)
C   B)  CHOLESKY FACTORIZATION OF THE BLOCK TRI-DIAGONAL PORTION
C       OF MATRIX A.
C  SEE PROG1A FOR PROGRAM SET-UP ASSOCIATED WITH EACH OF
C  THE TEST PROBLEMS.
C  SEE PROG2, GENA, BDIAG AND GETEG2 FOR MORE DETAILS.
C
      REAL A(5000),B(1024),W(1024,3),W1(1024,3)
      INTEGER INI(2000),INJ(5000),IK(1024,2),IW(1024)
C
      COMMON/MA31J/LROW,LCOL,NCP,ND,IPD
      COMMON/MA31N/MITE,ACC,EL,ER
      COMMON/MA31L/EPSTOL,U
      COMMON/MA31I/DD,LP,MP
      COMMON/MA31M/NI,NJ,NVERSN,NTYPE
C
      DATA U,EPSTOL/1.0E2,2.0E-6/
      DATA MITE,ACC,EL,ER/750,1.0E-2,0.0,1.2/
      DATA IAI,IAJ,ND/2000,5000,1024/
      DATA DD,LP,MP/1.0,6,5/
      DATA NI,NJ/32,32/
      DATA NVERSN,NTYPE/1,1/
C
      CALL GENA(ND,NZ,A,INI,INJ,IAI,IAJ,W,B,IK,IW)
      NZ1=NZ+1
      CALL BDIAG(ND,NZ,A,INI,INJ,A(NZ1),INJ(NZ1),IK,IW,
     *W(1,1),W(1,2))
      IAJ2=NZ+LROW
      CALL GETEG2(ND,NZ,A,INI,INJ,NZ,IAJ2,W,IK)
C
      END
```

```
      PROGRAM PROG2C(OUTPUT,DATA,TAPE5=OUTPUT,TAPE6=DATA)
C
C  DRIVER PROGRAM USED DURING PHASE III.
C  DESIGNED TO FIND THE EXTREME EIGENVALUES OF THE
C  SYMMETRICALLY PRECONDITIONED TEST MATRICES.
C  IT USES:
C   A)  2 LINE RED/BLACK GRID POINT ORDERING SCHEME (NTYPE = 3)
C   B)  REDUCED BLOCK INCOMPLETE CHOLESKY FACTORIZATION WITH
C       0 DIAGONALS ADDED AS PERFORMED BY SUBROUTINE RBIC0.
C  SEE PROG1A FOR PROGRAM SET-UP ASSOCIATED WITH EACH OF THE
C  TEST PROBLEMS.
C  SEE PROG2, GENA, RBIC0 AND GETEG2 FOR MORE DETAILS.
C
      REAL A(5000),B(1024),W(1024,3),W1(1024,3)
      INTEGER INI(2000),INJ(5000),IK(1024,2),IW(1024)
C
      COMMON/MA31J/LROW,LCOL,NCP,ND,IPD
      COMMON/MA31N/MITE,ACC,EL,ER
      COMMON/MA31L/EPSTOL,U
      COMMON/MA31I/DD,LP,MP
      COMMON/MA31M/NI,NJ,NVERSN,NTYPE
C
      DATA U,EPSTOL/1.0E2,2.0E-6/
      DATA MITE,ACC,EL,ER/1500,1.0E-2,1.0,0.0/
      DATA IAI,IAJ,ND/2000,5000,1024/
      DATA DD,LP,MP/1.0,6,5/
      DATA NI,NJ/32,32/
      DATA NVERSN,NTYPE/1,3/
C
      CALL GENA(ND,NZ,A,INI,INJ,IAI,IAJ,W,B,IK,IW)
      NZ1=NZ+1
      NCP=NJ
      CALL RBIC0(ND,NZ,A,INI,INJ,A(NZ1),INJ(NZ1),IK,IW,
     *W(1,1),W(1,2))
      IAJ2=NZ+LROW
      CALL GETEG2(ND,NZ,A,INI,INJ,NZ,IAJ2,W,IK)
C
      END
```

```
      PROGRAM PROG2D(OUTPUT,DATA,TAPE5=OUTPUT,TAPE6=DATA)
C
C  DRIVER PROGRAM USED DURING PHASE III.
C  DESIGNED TO FIND THE ESTREME EIGENVALUES OF THE
C  SYMMETRICALLY PRECONDITIONED TEST MATRICES.
C  IT USES:
C   A) NATURAL GRID POINT ORDERING SCHEME (NTYPE = 0)
C   B) NO PRECONDITIONING
C  SEE PROG1A FOR PROGRAM SET-UP ASSOCIATED WITH EACH  OF
C  THE TEST PROBLEMS.
C  SEE PROG2, GENA AND GETEG2 FOR MORE DETAILS.
C
      REAL A(5000),B(1024),W(1024,3),W1(1024,3)
      INTEGER INI(2000),INJ(5000),I(104,2),IW(1024)
C
      COMMON/MA31J/LROW,LCOL,NCP,ND,IPD
      COMMON/MA31N/MITE,ACC,EL,ER
      COMMON/MA31L/EPSTOL,U
      COMMON/MA31I/DD,LP,MP
      COMMON/MA31M/NI,NJ,NVERSN,NTYPE
C
      DATA U,EPSTOL/1.0E2,2.0E-6/
      DATA MITE,ACC,EL,ER/750,1.0E-2,0.0,1.2/
      DATA IAI,IAJ,ND/2000,5000,1024/
      DATA DD,LP,MP/1.0,6,5/
      DATA NI,NJ/32,32/
      DATA NVERSN,NTYPE/1,0/
C
      CALL GENA(ND,NZ,A,INI,INJ,IAI,IAJ,W,B,IK,IW)
      LROW=0
      DO 10 I=1,ND
      IK(I,1)=0
      IK(I,2)=I
      W(I,2)=1.0
   10 CONTINUE
C
      WRITE(LP,15)
   15 FORMAT(19H NO PRECONDITIONING)
      IAJ2=NZ+LROW
      CALL GETEG2(ND,NZ,A,INI,INJ,NZ,IAJ2,W,IK)
C
      END
```

```
      SUBROUTINE GETEG2(NN,NZ,A,INI,INJ,IAI,IAJ,W,IK)
C
C  SUBROUTINE TO CALCULATE THE HIGH AND LOW ORDER
C  EIGENVALUES OF OUR SYMMETRICALLY PRECONDITIONED
C  INPUT MATRIX USING THE HARWELL EA14A LANCZOS
C  ALGORITHM.  SEE SOLVE FOR DESCRIPTION OF INPUT
C  PARAMETERS.
C
      REAL A(IAJ),W(NN,3)
      REAL EIG(1024),U(1024),V(1024),T1(1024),T2(1024)
      REAL X(3000),DEL(3000),ALFA(5000),BETA(5000)
      INTEGER INI(IAI),INJ(IAJ),IK(NN,4)
      INTEGER NU(3000)
C
      COMMON/EA14BD/PRVT(4),IPRVT(6)
      COMMON/MA31I/DD,LP,MP
      COMMON/MA31J/LROW,LCOL,NCP,ND,IPD
      COMMON/MA31N/MITE,ACC,EL,ER
C
      DATA LEIG,LX,LALFA/1024,3000,5000/
C
      NZ1=NZ+1
      IAJ1=IAJ-NZ
      IFLAG=-1
      CALL SECOND(TIM1)
C
C  PASS 1 CALCULATES THE EIGENVALUES IN THE INTERVAL
C     EL TO ER AS SPECIFIED BY THE CALLING ROUTINE.
C  PASS 2 CALCULATES THE HIGH ORDER EIGENVALUES USING
C     ESTIMATED NORM OF THE MATRIX PRODUCED BY ROUTINE
C     EA14A TO DEFINE THE INTERVAL TO BE EXAMINED.
C
      DO 290 IPASS=1,2
C
      WRITE(MP,10) IPASS
   10 FORMAT(6H PASS ,I1,6H START)
C
      CALL SECOND(TIM2)
C
C  A MAXIMUM OF MITE ITERATIONS ARE ATTEMPTED TO
C  ACQUIRE ALL EIGENVALUES IN THE INTERVAL EL TO ER
C  TO AN ACCURACY OF ACC.
C
      DO 30 ITER=1,MITE
C
      CALL EA14AD(NN,EL,ER,ACC,LEIG,LX,LALFA,LP,IFLAG,
     *U,V,EIG,NEIG,X,DEL,NU,ALFA,BETA)
C
```

```
            IF (IFLAG.EQ.0) GO TO 200
   50       IF (IFLAG.GT.1) GO TO 100
      C
      C  CALCULATES VECTOR U = VECTOR U + MATRIX A' TIMES VECTOR V,
      C  WHERE MATRIX A' IS THE RESULT OF SYMMETRICALLY
      C  PRECONDITIONING MATRIX A BY MATRIX C.
   55 C
            CALL MA31G2(NN,A(NZ1),INJ(NZ1),IAJ1,W(1,2),IK,V,T1)
            CALL MA31H(A,W,INI,INJ,NZ,NN,T1,T2)
            CALL MA31G1(NN,A(NZ1),INJ(NZ1),IAJ1,W(1,2),IK,T2)
      C
   60       DO 20 I=1,NN
            U(I)=U(I) + T2(I)
       20   CONTINUE
      C
       30   CONTINUE
   65       GO TO 180
      C
      C  EA14AD IS SIGNALING FAILURE
      C
       100  WRITE(LP,110) IFLAG
   70       WRITE(MP,110) IFLAG
       110  FORMAT(26H0EA14AD HAS FAILED. IFLAG=,I2)
            GO TO 290
      C
      C  EA14AD COULDN'T FINISH IN THE REQUESTED
   75 C  NUMBER OF ITERATIONS
      C
       180  WRITE(LP,185) MITE
            WRITE(MP,185) MITE
       185  FORMAT(39H0--WARNING ALL EIGENVALUES NOT FOND IN,
   80      *I4,2X,10HITERATIONS)
            ITER=MITE
      C
      C  OUTPUT DATA ON THE CALCULATED EIGENVALUES
      C
   85   200  CONTINUE
            CALL SECOND(TIM3)
            TRUN=TIM3-TIM2
            WRITE(LP,202) IPASS,TRUN
       202  FORMAT(6H PASS ,I1,12H RUN TIME = ,F10.3,5H SECS)
   90       WRITE(LP,205) PRVT(1)
       205  FORMAT(19H0SPECTRAL RADIUS = ,E14.7)
            WRITE(LP,210) EL,ER
       210  FORMAT(19H INTERVAL EXAMINED ,E13.5,3H - ,E13.5)
            WRITE(LP,215)
   95   215  FORMAT(30H0DATA ON RESULTING EIGENVALUES)
            WRITE(LP,220) ITER,ACC
```

```
 220  FORMAT(8H ITER = ,I3,2X,6HACC = ,E13.5)
      WRITE(LP,230) NEIG
 230  FORMAT(28H NUM DISTINCT EIGENVALUES = ,I3)
100   C
      WRITE(LP,235)
 235  FORMAT(28HOORDERED LIST OF EIGENVALUES)
      WRITE(LP,240) (EIG(I),I=1,NEIG)
 240  FORMAT(1X,10E13.5)
105   WRITE(MP,245) IPASS
 245  FORMAT(6H PASS ,I1,5H DONE)
      C
      C PERPARE TO EXAMINE EIGENVALUES AT THE END OF THE SPECTRUM.
      C
110   EL=PRVT(1)*0.8
      ER=PRVT(1)*1.1
      C
      C
 290  CONTINUE
115   C
      CALL SECOND(TIM4)
      TT=TIM4-TIM1
      WRITE(LP,295) TT
 295  FORMAT(18H TOTAL RUN TIME = ,F10.3,5H SECS)
120   C
      RETURN
      END
```

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